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PARALLEL RADIATION TRANSPORT CODE  
A MONTE CARLO METHOD  
APPLIED TO ILLIAC IV  
AND ITS STATISTICAL CONSIDERATION

by

Ken'ichi Miura

October 1, 1971



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## Abstract

A Monte Carlo method to solve radiation transport problems by using the ILLIAC IV is discussed. An emphasis is put on the special features to be encountered in parallel computation: data structure, PE efficiency, etc. A test program implemented in GLYPNIR--an ILLIAC IV language--is shown and some preliminary results on its statistical properties are also discussed.



## ACKNOWLEDGEMENTS

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## 1. INTRODUCTION

The Monte Carlo Method started its history in 1777 when Conte de Buffon (1707-1788) presented a famous problem to calculate  $\pi$  by tossing needles (Buffon's problem). (Ref. [1] ). Real progress was not made until digital computers became available. In 1947 J. von Neumann, R. Richtmyer and S. Ulam used the ENIAC to solve neutron diffusion problems by simulating the movement of particles. (Ref. [12]). Since then, development has been remarkable in fields such as partial differential equations, definite integrals, serving systems, linear equations and transport problems. (Ref. [10] ). In transport problems a necessity to calculate neutron flux within reactors or gamma-ray flux through shielding walls has encouraged the development of more efficient algorithms.

Due to their statistical nature, simulation of random processes on a digital computer requires a large memory and fast logical and arithmetic operations to obtain necessary accuracy. The parallel structure of the ILLIAC IV computer, although originally designed for matrix problems or partial differential equations, is applicable to random simulation. This paper is concerned with the application of the ILLIAC IV to radiation transport problems.

In this chapter, a physical model and the basic equations are presented. Certain other assumptions are also discussed. Special features to be encountered in parallel computation will be discussed in the subsequent chapters.

### 1.1 Basic Equations

The physical phenomenon described in this paper is "non-linear radiation transport" in the low energy region, which is encountered, for example, in the study of stellar atmosphere. (Ref. [2], [4], [7]).

Consider a block of material (or gas, to be referred to as "medium" hereafter) which is not necessarily homogeneous. Let a beam of photons be incident on it (or let a heat source be attached to it). Some of the photons will pass through the medium undisturbed, some will be absorbed by the medium and release their energy to it, while others will be scattered into new directions (with new energies). Since the absorption of photons affects the local temperature and the change of the temperature itself affects the emission of photons, the whole process is rather complicated. Evolution of the photon intensity and the temperature is given in the form of a system of nonlinear integro-differential equations as will be shown below.

Let  $dE$  denote the radiation energy in a frequency range  $(\nu, \nu + d\nu)$  which is transported across an element of area  $dS$  at  $x$  and in directions confined to a solid angle  $d\Omega$  during a time  $dt$ . (Fig. 1.1). Then the intensity  $I(\vec{x}, \mu, \nu)$  is defined as follows:

$$dE_{\nu} = I(\vec{x}, \mu, \nu) \cos \theta \, d\nu \, dS \, d\Omega \, dt$$

The basic equation which  $I$  satisfies is:

$$\begin{aligned} \frac{d}{ds} I(\vec{x}, \mu, \nu) = & -\sigma_{\text{tot}} I(\vec{x}, \mu, \nu) + B(\vec{x}, \mu, \nu) \\ & + \sigma_{\text{scatt}} \cdot \iint P(\mu \rightarrow \mu') I(\vec{x}, \mu', \nu) d\mu' d\Omega \end{aligned} \quad (1,1)$$

The left hand side of (1,1) is the total change of the intensity along the path of radiation; its more explicit form is dependent on the geometry



which one is to consider (Cartesian, spherical, etc.). Table 1.1 shows some examples.

The first term on the right hand side represents diminution of the radiation caused by various kinds of interaction: absorption, scattering, or pair-creation (only in high energy region). The probability of the occurrence of each interaction is expressed in terms of cross section.  $\sigma_{\text{tot}}$  is the total cross section and of course  $\sigma_{\text{tot}} = \sigma_{\text{abs}} + \sigma_{\text{scatt}} + \dots$ . The second term is the source term which includes the black body radiation (note that the absorption of photons causes re-emission of new photons through this process), pair-annihilation (only in high energy region) and some other heat sources. In astrophysics, the assumption of local thermodynamical equilibrium is often adopted. That is, if the temperature in the medium varies very slowly with relation to position then the laws of thermodynamic equilibrium are still applicable at each point with the local temperature. Therefore, photons are re-emitted according to "Kirchhoff's law:"

$$B(\vec{x}, \mu, \nu) = \sigma_{\text{abs}} \cdot \frac{2h\nu^3}{c^2} \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

where  $\sigma_{\text{abs}}$  and  $T$  depend on  $\vec{x}$ .

Note that the temperature  $T$  is involved in a non-linear way.

The third term is the scattering term and represents a contribution from other directions  $\mu'$  into  $\mu$ .  $P$  denotes the scattering probability from  $\mu'$  to  $\mu$ . If Thomson scattering is assumed, then

$$P(\cos \theta) = \frac{3}{16} (1 + \cos^2 \theta)$$

and

$$\mu' = \mu \cdot \cos \theta - \sqrt{1-\mu^2} \sin \theta \cos (\psi' - \psi)$$

(See Fig. 1.2)

The temperature  $T$ , on the other hand, changes with time according to the following equation:

$$\rho C_v \frac{\partial T}{\partial t} = \frac{2h}{c^2} \int_0^\infty \sigma_{abs} v^3 \cdot \frac{(-1)}{\exp\left(\frac{hv}{kT}\right) - 1} dv$$

where

$$+ \int_{-1}^1 dv \int_0^\infty \sigma_{abs} \cdot I(\vec{x}, \mu, \nu) d\nu \quad (1,2)$$

$\rho$  : density

$C_v$  : specific heat

$\sigma_{abs}$  : absorption cross section  
(dependent on  $\vec{x}$  and  $T$  also depends on  $\vec{x}$ )

The left hand side of (1,2) is the change of stored energy in the medium. The first term on the right hand side is the loss of energy due to the black body radiation. The second term is the gain of energy due to the absorbed photons. Hence, (1,1) and (1,2) describe the energy balance of the total system. (Fig. 1.3). If  $I$  is averaged over frequency, then those equations become simpler. That is,

$$\frac{d}{ds} I(\vec{x}, \mu, t) = - (\sigma_{abs} + \sigma_{scatt}) I(\vec{x}, \mu, t) + \sigma_{scatt} \int_{-1}^1 I(\vec{x}, \mu', t) P(\mu, \mu') d\mu' + \sigma_{abs} \frac{\sigma_{stephan}}{\pi} T(\vec{x}, t)^4 + S(\vec{x}, \mu) \quad (1,1)'$$

and

$$\rho C_v \frac{\partial T(\vec{x}, t)}{\partial t} = - \sigma_{abs} \frac{\sigma_{stephan}}{\pi} T(x, t)^4 + \sigma_{abs} \int_{-1}^1 I(\vec{x}, \mu', t) d\mu' \quad (1,2)'$$

## 1.2 The Model for Monte Carlo Calculation (general discussion)

This section describes the model implemented on ILLIAC IV.

(1) The geometry is two dimensional. (Density is assumed to be uniform with regard to the third coordinate although particles

travel in three dimensional space).

(2) The material is expressed as 64 x 8 cells (it is easy to extend up to 64 x 64); each cell can have variable density and specific heat.

(3) Absorption is due to the photo-electric effect, and its cross section can be factored as a density dependent term and another term which is dependent on photon energy. The same thing is assumed as for scattering cross section.

$$\sigma_{\text{abs}} = \rho(x,y) \cdot \kappa(E)$$

$$\sigma_{\text{scatt}} = \rho(x,y) \cdot \lambda(E)$$

$\rho(x,y)$ ,  $\kappa(E)$  and  $\lambda(E)$  can be stored as tables and linear interpolation is used to generate cross sections.

(4) The number of particles which are to be created is dependent on the local temperature. There are two alternatives as to their energies: Planckian distribution or mono-energetic (the latter is adopted for the test program).

Photons are modeled as a particle table. The term "particles" should be distinguished from "photons" hereafter. The former means pseudo-photons within a computer whereas the latter means actual photons. The table size is limited by the size of memory available. Refer to Chapter 3 for the actual table size. The medium has been divided into small cells of  $\Delta x \cdot \Delta x$ . The time unit is  $\Delta t$ .

### 1.3 Creation of Particles

At the beginning of a time step, the number of particles to be created in cells is determined according to the temperature. As the table size is limited, more particles are assigned to those cells which are hot. Therefore, only the cell numbers are assigned to the new particles at this

stage.

The creation of new particles follows. The quantities given below are assigned to each of the new particles:

- (1) relative coordinates  $x$  and  $y$  . . . .(uniformly distributed)
- (2) direction cosine  $\mu$  . . . . .(uniformly distributed)
- (3) sine and cosine of azimuthal angle .(uniformly distributed)
- (4) survival distance (path length). . .(exponentially distributed)
- (5) fraction  $\xi$  to indicate at what time  $\xi\Delta t$  this particle was created. . . . .(uniformly distributed)

#### 1.4 Processing a Time Step

After all the new particles are created, the table scanning starts. The position of a particle is incremented as follows:

$$x' = x + v\mu\Delta t$$

$$y' = y + v \sqrt{1-\mu^2} \sin \phi \cdot \Delta t$$

The distance which a particle is supposed to travel ( $l = v\Delta t$ ) is compared with  $\tau/\sigma_{\text{tot}}$  where  $\sigma_{\text{tot}} = \sigma_{\text{abs}} + \sigma_{\text{scatt}}$ , and if the former is larger than the latter an interaction is assumed to occur. The type of interaction is determined by generating a uniformly distributed random number and comparing it with  $\sigma_{\text{abs}}/\sigma_{\text{tot}}$ . If the random number is less than this quantity, absorption is taken and the energy of the particle is added to the cell in which the interaction occurred. This particle is to be destroyed.

On the other hand, if the random number is greater than this quantity, then the interaction is scattering and new angles, new survival distances are selected and assigned to the particle.

### 1.5 The New Temperature

After the scanning of the particle table, the intensity in each cell is computed by summing the particles in it. Then the new temperature is computed.

The last three sections are a narrative description of the Monte Carlo program. A flow chart of the computation process (not the program) is shown in Figure 1.4. In the subsequent chapters particular problems for parallel processing are to be discussed.

Table 1.1

$$\frac{d}{ds} = \frac{1}{c} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial x} \quad (\text{slab-symmetry})$$

$$\frac{1}{c} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial}{\partial \mu} \quad (\text{spherical symmetry})$$

$$\frac{1}{c} \frac{\partial}{\partial t} + \sin \phi \left( \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r} \right) + \cos \phi \frac{\partial}{\partial z} \quad (\text{cylindrical symmetry})$$

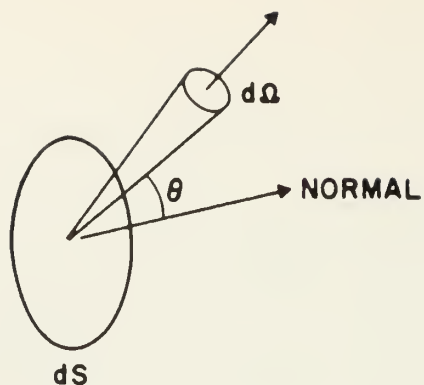


Figure 1.1 Definition of Intensity

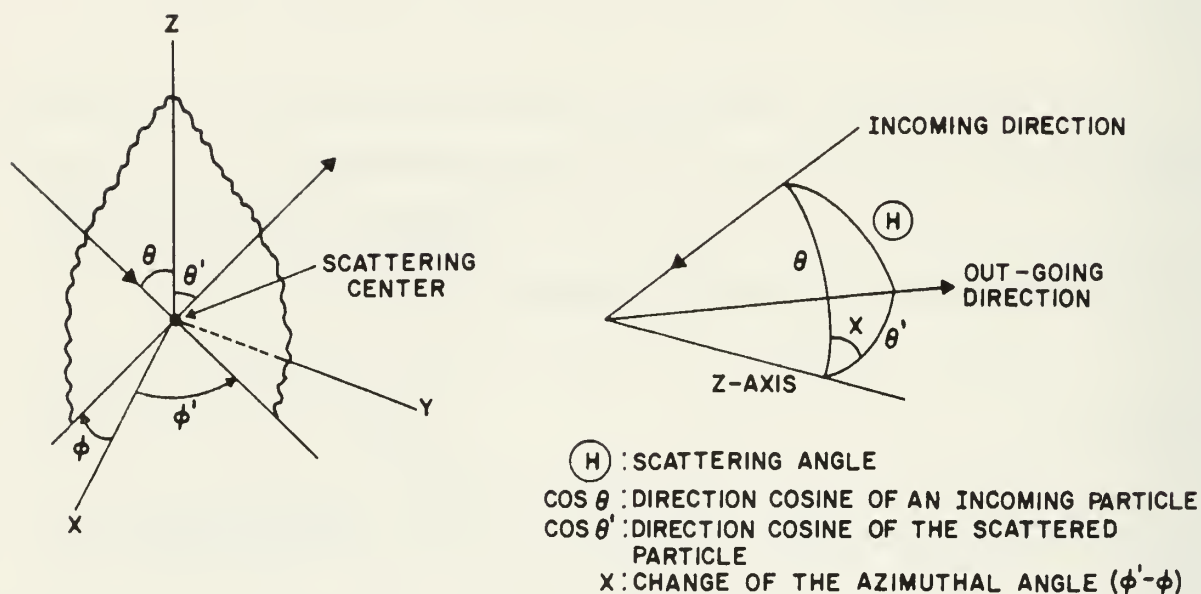
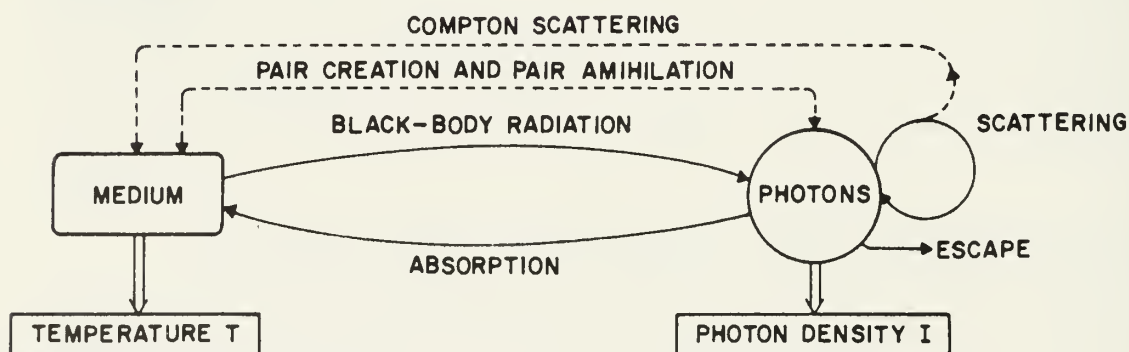


Figure 1.2 Definitions of Angles in Scattering Process

Figure 1.3 Flow Diagram of Conversion of Energy  
(Dotted lines are for high energy case)



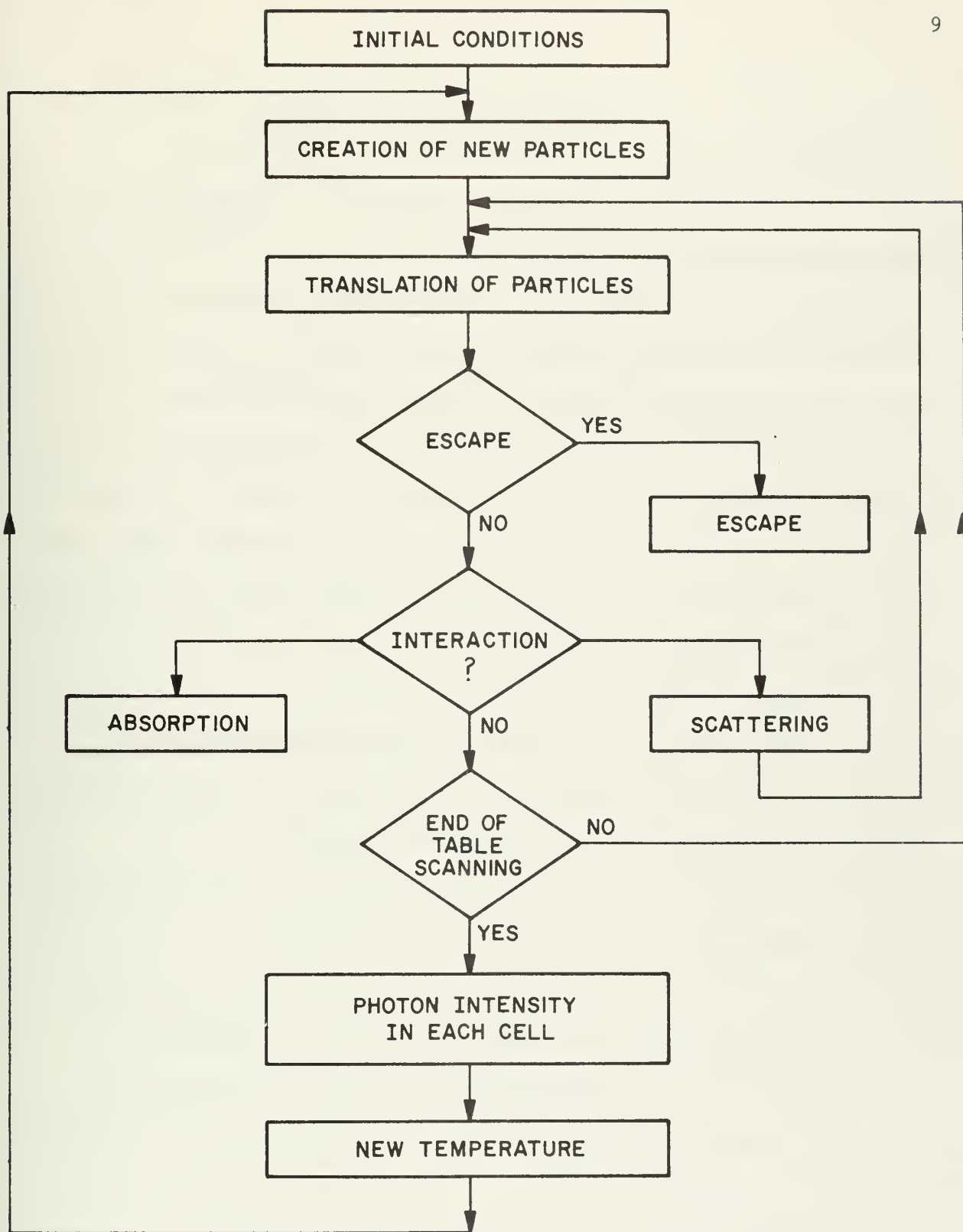


Figure 1.4 A Flow Chart of a Monte Carlo Program

## 2. RANDOM SAMPLING

An important part of a Monte Carlo method is the generation of good random numbers. The generation of uniformly distributed random numbers is discussed in Section 2.1. Transformation from the uniform distribution to an arbitrary distribution is discussed with some examples which are encountered in transport problems (Sections 2.2 and 2.3). In this and subsequent chapters, an emphasis is put on the application of the Monte Carlo method to the ILLIAC IV computer, and readers are assumed to have a fundamental knowledge of it (especially its architecture). (Ref. [11]). Terms such as PE (the processing element), CU (the control unit) will be used.

### 2.1 Linear Congruential Method

Since von Neumann's middle-square method several methods have been investigated to generate uniformly distributed random numbers. (Ref. [6]). The linear congruential method is generally accepted to be the best for digital computers for the following reasons:

- (1) it is easy to calculate the subsequent random number from the updated one,
- (2) only a very small space in the memory is required (unlike storing the entire or partial table of random numbers),
- (3) repeated reproduction of the same sequence is possible,
- (4) the period of random sequence is long (if proper coefficients are chosen).

The linear congruential method can be described by the following formula:

$$X_{n+1} = (AX_n + C) \bmod T \quad (2,1)$$

where A and C are constants,  $X_n$  is the  $n$ th random number and T is also a constant. The initial value  $X_0$  is given.  $X_n$  ranges between 0 and T.  $K_n = X_n/T$  ranges in (0,1). The method is called multiplicative if  $C = 0$ . Otherwise, it is called mixed congruential. T is usually chosen to be the register length of the computer ( $2^{48}$  in ILLIAC IV). A and C must be such that  $X_n$  yields good uniform random sequence. Consult reference [6] or [14] for detail, since the principle of this method is not to be presented in this paper. The method which has been adopted for the ILLIAC IV is the multiplicative congruential method (Ref. [14]) but it is also possible to use the mixed congruential method. In both methods the coefficients should be chosen to give the longest possible period of random sequence so that one sequence of random numbers can be decomposed into 64 sufficiently long subsequences. The easiest way is to divide the entire sequence into 64 subsequences and generate each subsequence in a different PE. The problem with this method is the serial correlations of random numbers across PEs or within each PE. For example, if each processor element starts with every  $2^{20}$  random number of the original sequence then the correlations of random numbers separated by distance  $2^{20}$  or its multiples must be closely examined, because they will be generated simultaneously in PEs and any non-negligible correlation among them could cause trouble. Nothing is known about the correlations over that long distance for the coefficients currently recommended for conventional machines. Usually serial correlations of distance up to 10 or 20 are examined. Therefore, closer attention must be paid to choosing proper coefficients.

There is a formula about the bound of serial correlation factor of any distance  $r$  (Ref. [5]):

$$\rho_r \leq \frac{A_r}{T} + \frac{1}{A_r} \left(1 - \frac{6C_r}{T} + 6 \left(\frac{C_r}{T}\right)^2\right) \quad (2,2)$$

$$\text{where } X_{s+r} = (A_r X_s + C_r) \bmod T$$

$$A_r = A^r \bmod T$$

$$C_r = C \cdot \frac{A^r - 1}{A - 1} \bmod T$$

$$\rho_r = \lim_{n \rightarrow \infty} \frac{\sum_{k=1}^{n-r} X_k \cdot X_{k+r} - \left(\sum_{k=1}^n X_k\right)^2}{\sum_{k=1}^n X_k^2 - \left(\sum_{k=1}^n X_k\right)^2}$$

$A_r \approx \sqrt{T}$  in (2,2) yields the smallest serial correlation factor  $\rho_r$  in mixed congruential methods. But it is impossible to choose  $A$  so that  $A_1, A_2, \dots$  all become the order of  $\sqrt{T}$ . Therefore, an actual test run in each case is necessary. Refer to a document to be published in the future for the result of the example given in Reference [14]. ( $A=5^{17}$ ,  $C=0$ ,  $T=2^{48}$ ).

The method to use--multiplicative or mixed--is another problem. Statistical tests have shown that the multiplicative method is better than the mixed. (Ref. [9]). The advantage of the mixed method is that all the integers between 0 and  $T$  are covered so that sequence can be started at any number. In the multiplicative method, on the other hand, the initial random number must be chosen very carefully. The actual algorithm used for the computation on ILLIAC IV will be given in a document to be published.

## 2.2 Random Sampling from a Given Distribution Function

There are several methods to sample random numbers of a given distribution of uniform random numbers.

### 2.2.1 Rejection Method

The rejection method was proposed by von Neumann and was used in his works on neutron transport simulation. (Ref. [13]). Theoretically, this method can be applied to any type of density function. It is not efficient, however,

for the functions which have sharp maxima. In those cases many random numbers are wasted and as a consequence the number of trials increases. If a density function has a domain  $[a,b]$  and maximum value  $f_{\max}$ , the rate of success is  $1/(f_{\max} \times (b - a))$ . (Fig. 2.1). This disadvantage is disastrous if the method is applied in a straightforward way to parallel sampling, since one cannot proceed to the next step until all the PEs accept random numbers.

Suppose, for example, that there are  $N$  PEs, each of which samples a random number in parallel using the rejection method. Let  $p$  denote the probability of accepting a random number in a PE in each individual trial, i.e.  $p = 1/(f_{\max} \times (b - a))$ . Then the probability that each PE has accepted at least one random number after  $r$  trials is

$$P(p, r, N) = \{1 - (1 - p)^r\}^N \quad (2,3)$$

This can be shown very easily because  $(1 - p)^r$  is the probability that none of the  $r$  trials are successful for individual PE.

Take Planckian case, for example. Then

$$f(x) = \frac{15}{4\pi} \cdot \frac{x^3}{\exp(x) - 1} \quad f_{\max} = .23$$

$$f(10) = .8 \times 10^{-2} \quad \therefore F(10) \approx 1 \quad (\text{Take } b = 10 \text{ and } a = 0)$$

$$\text{then } p = 1/(.23 \times 10) = .435$$

with  $N = 64$  (ILLIAC IV),

$$P(.435, r, 64) = \{1 - (.565)^r\}^{64}$$

Several curves are plotted in Figures 2.2 and 2.3. Figure 2.2 shows a rapid fall-off of the efficiency with the decrease of  $p$ .

As models become more complicated, various kinds of distribution functions will appear to determine scattering angles for high energy particles (Klein-Nishina's formula) or pair creations followed by reannihilation

etc. Each of these processes contains several branches in itself; overall efficiency is not high. Table 2.1 shows some examples taken from Reference [15]. Efficient implementation of these processes using the rejection method for the ILLIAC IV is very difficult.

### 2.2.2 Method of Inverse Function

If a distribution function  $F$  has an inverse function  $F^{-1}$  which is not complicated to evaluate, then a random number  $x$  can be sampled from  $f=F'$  according to the following formula:

$$R = \int_{-\infty}^x f(x') dx'$$

$$\text{or } x = F^{-1}(R)$$

where  $f$  is a density function, and  $R$  is a uniformly distributed random number

The advantage of this method is that all the PEs can produce random numbers simultaneously. But this advantage will be cancelled out if  $F^{-1}$  is very complicated and takes a long time to evaluate. Exponential distribution is a typical example for use of this method:

$$f(x) = \lambda \exp(-\lambda x), \quad x = 1/\lambda \log(1-R)$$

where  $R$  is a sampled uniform random number.

### 2.2.3 Approximation of Distribution Functions by some Simpler Ones

If the inverse of distribution functions cannot be obtained explicitly, or are not simple to calculate, they are approximated by some simpler functions, or more frequently by a set of data points. The latter is essentially equivalent to the inverse linear interpolation with table lookup technique.

The method can be described as follows:

The region  $(0,1)$  on the ordinate (i.e., accumulated distribution function) is divided into  $N$  equal subintervals. Then a uniform random number  $R$  is



sampled and the interval in which it is located is checked. A random number  $X$  with required distribution  $f$  is calculated by using ordinates and abscissas of the two points which are the edges of the selected subintervals, i.e., if  $F_k < R < F_{k+1}$ , then  $x = \frac{(F_{k+1} - R) \cdot X_k + (R - F_k) \cdot X_{k+1}}{F_{k+1} - F_k} =$

$$X_k(k + 1 - N \cdot R) + X_{k+1}(N \cdot R - k) \quad (2,4)$$

The basic idea of this method is to chop the graph of a given probability distribution function  $f$  into  $N$  strips of equal area and approximate  $f$  by the average  $f_k$  in each interval so that  $f_k \cdot (X_{k+1} - X_k) = 1/N$ . (Fig. 2.4). Obviously the accuracy is good near maximum point of  $f$  where the width of the strip is relatively narrow. On the other hand, it is not good in the region where  $f$  is close to zero (e.g. edge regions of Gaussian or Planckian type distributions). Figure 2.5 shows an example of Planckian distribution. (Sampling number = 10,000,  $N = 32$ ).

Sometimes a density function contains a parameter  $\mu$ . Consider the following example:

$$F(x, \mu) = 1/8 \{ (3 - \mu^2)x + (\mu^2 - 1/3)x^3 \} \quad 0 \leq x, \mu \leq 1 \quad (2,5)$$

which is used to determine a new direction cosine  $x$  from an old one,  $\mu$ , in one dimensional radiative transport problems. Interpolation in this case involves two variables,  $x$  and  $\mu$ . Data is stored as a reference table; they are values  $x(k, m)$  ( $0 \leq k, m \leq n$ ), which satisfy  $F(x(k, m), \mu_m) = k/N$  ( $0 \leq k, m \leq 1$ ). A random number  $x$  for given  $\mu$  is then calculated by:

$$\begin{aligned} X(\mu) &= (\mu_{m+1} - \mu) X(\mu = \mu_m) + (\mu - \mu_m) X(\mu = \mu_{m+1}) \\ &= X(k, m)(k+1 - N \cdot R)(m+1 - \mu \cdot N) + X(k, m+1)(k+1 - N \cdot R)(\mu \cdot N - m) + X(k+1, m) \\ &\quad (N \cdot R - k)(m+1 - \mu \cdot N) + X(k+1, m+1)(N \cdot R - k)(\mu \cdot N - m) \text{ where } \mu_m < \mu < \mu_{m+1}, \\ X(i, j) &= F^{-1}(i/N, \mu_j) \text{ and } k, m \text{ are chosen so that } (R, \mu) \text{ in } X-\mu \end{aligned}$$

plane is inside a trapezoid formed by four points  $(X(k,m),m), (X(k+1,m),m), (X(K,m+1),m+1)$ , and  $(X(K+1,m+1),m+1)$ .

More precisely, linear interpolation is first applied to the two planes  $\mu = \mu_m$  and  $\mu = \mu_{m+1}$  separately, then the two lines obtained as a result are used to get the ultimate interpolation line which is parallel to the  $x = \text{constant}$  plane and on which the point in question is located. Therefore, the following errors must be taken into account:

$$|E_m| \leq \max_{(x_k, x_{k+1})} \left| \frac{\partial^2 f}{\partial x^2} \right|_{\mu=\mu_m} \cdot (x_{k+1} - x)(x - x_k) / 2,$$

$$|E_{m+1}| \leq \max_{(x_k, x_{k+1})} \left| \frac{\partial^2 f}{\partial x^2} \right|_{\mu=\mu_{m+1}} \cdot (x_{k+1} - x)(x - x_k) / 2,$$

$$|E_m| = \max(|E_m|, |E_{m+1}|),$$

$$|E_x| = \max_{(\mu_m, \mu_{m+1})} \left| \frac{\partial^2 f}{\partial \mu^2} \right|_{x=x} \cdot (\mu_{m+1} - \mu)(\mu - \mu_m) / 2,$$

$$E_{\text{tot}} \leq E_m + E_x \leq (h^2 M + k^2 M') / 8 \quad (2,7)$$

where

$$h = (x_{k+1} - x_k)$$

$$k = \mu_{m+1} - \mu_m$$

$$M = \max \left| \frac{\partial^2 f}{\partial x^2} \right| (X_k \leq X \leq X_{k+1}, \mu_m \leq \mu \leq \mu_{m+1})$$

$$M' = \max \left| \frac{\partial^2 f}{\partial \mu^2} \right| (X_k \leq X \leq X_{k+1}, \mu_m \leq \mu \leq \mu_{m+1})$$

Example:  $N = 32$

$$F = \{ (3 - \mu^2) \cdot x + (\mu^2 - 1/3)x^3 \} \cdot 3/8$$

$$M = 3/2 \quad (0 \leq x, \mu \leq 1)$$

$$N = \sqrt{3}/6 \quad (0 \leq x, \mu \leq 1)$$

$$\therefore E_{\text{tot}} \leq 1/8 \cdot 1/1024 \cdot (3/2 + \sqrt{3}/6)$$

$$\approx 2.2 \cdot 10^{-5}$$

This method is good when memory size is not valuable compared with the number of arithmetic operations or when  $F(x, \mu)$  is very complicated to evaluate.

#### 2.2.4 Root-finding Method

Sometimes formulae for functional iteration (such as Newton's formula) are useful to generate random numbers.

Suppose the probability density function is  $p(x)$  and its accumulated distribution function is  $F(x)$ . If a random number  $R$  is sampled out of a uniform population in  $[0,1]$ , then  $F(x) - R = 0$  when solved for  $x$ , yields a random sample from  $p(x)$ . Several iterations of Newton's method are enough to get a satisfactory result if  $F(x)$  is not too ill-behaved.

It is very important in parallel computation that all PEs get accurate values after a certain number of iterations, regardless of the distribution of  $R$ s. (Note that all PEs have different  $R$ s). In the ILLIAC IV, any logical decision which involves the CU (control unit) takes a long time and is desirable to avoid. The following illustrates this. To determine a scattering angle in Thomson scattering,  $p(x) = 3/4 (1 + x^2)$  ( $0 \leq x \leq 1$ ). Hence  $F(x) = 3/4 (x + \frac{x^3}{3})$  and Newton's formula to calculate a

next approximation is:

$$X_{n+1} = X_n - \frac{F(X_n)}{f(X_n)} = \frac{4/3 \cdot R + \frac{X_n^3}{2}}{1 + X_n^2} \quad (2,8)$$

$X_0 = .7$  turned out to be the best as the initial value; three iterations give satisfactory results ( $< 10^{-8}$ ), whatever  $R$  may be.

In general, this method is not very efficient if evaluation of the right hand side of (2,8) requires much computation; i.e., some transcendental functions such as exponential or sine are involved. The third method and

the fourth method of this section are complimentary to each other in a sense. Note that both the root-finding and the inverse function method share an advantage over the interpolation method. They require less memory space.

## 2.3 Some Remarks on Random Sampling

### 2.3.1 Forcing (sampling exactly n samples out of N)

Forcing is one of the techniques to reduce the variance of sampling. Suppose 10% of samples out of a population which contains  $N$  elements are selected. The simplest way is to generate random numbers  $R$  and compare them with 0.1. If  $R \leq 0.1$  at the  $K$ th trial then select the  $K$ th element. Thus at the end of  $N$  trials,  $0.1N$  samples on the average will be obtained. But sometimes exactly  $0.1N$  samples might be needed.

The alternative method is to keep changing the criterion at each step so that exactly  $0.1N$  samples can be obtained at the end. This is shown in Reference [6], for example. The probability of selecting the  $K - 1$ st element is  $\frac{0.1N - n}{N - k}$  if  $n$  samples have already been sampled in the  $K$  steps.

This method is applicable to the ILLIAC IV in the usual way within PEs. It is difficult, however, to apply it to select exactly  $n$  PEs out of 64, although this kind of problem may be occasionally encountered. The reason is that the process is inherently sequential in the sense that the probability to pick up the  $t + 1$ st element is dependent on the number of elements selected so far. Therefore, an efficient parallel selection is difficult.

In the case in which the sampling criterion  $n$  is large it is possible to increase the efficiency by dividing 64 PEs into several sub-groups of the same number of PEs such as 4 groups of 16 PEs, and each group

selects  $n/4$  PEs randomly within itself. But the sampling is not free from biasing and it might cause trouble in some cases.

### 2.3.2 Shuffling (or random permutation of data)

Shuffling is also a task which is not easily adopted to the ILLIAC IV. Data can be shuffled in both ways--within PEs or across PEs. The former case causes no trouble and the algorithm to be stated below works in parallel, but one will encounter the same difficulty as with forcing in the latter case. There are two problems involved in the random permutation: (1) how to generate addresses to send data to and (2) how to send data actually. The first problem is equivalent to generating 64 random integers ( $0 \sim 63$ ) each of which is different from all others. If each PE generated a random integer independently of others, the probability of success is  $64!/64^{64} \sim e^{-64}$ . The algorithm suggested by Knuth (Ref. [6]) is applicable, but not efficient. It states:

Suppose the data are  $A(1)$  through  $A(N)$ . In the first step of the problem given above,  $A(i)$  is in the  $i - 1$ th PE and exchange of data is performed by means of the routing registers. Now, there is a register  $R$  which contains an integer. Initial value of  $R$  is  $N$ . Then a random integer  $S$  is generated which ranges from 1 to the content of  $R$ . Interchange  $A(S)$  with  $A(R)$ . Decrease the content of  $R$  by 1. Generate  $S$ , interchange, . . . and so forth. This process is continued until  $R$  becomes 1.

Obviously, the method is sequential and 64 pairs of routing (forward and backward) are necessary.

The second step of the given problem (namely, sending data to a specified address) is a special case of the table lookup method, in which the one-to-one correspondence between the sources and destinations is guaranteed. The only conceivable method is to use the routing register as

"conveyer" to put all the data on and to drop the appropriate data to their destinations after each routing of distance 1. This takes 64 routings in the worst case.

Table 2.1

Type of Processes	$n^{(1)}$	$p = n^{-1(2)}$	$b^{(3)}$
exponential distribution	4.3		3
$\sin\phi$ and $\cos\phi$ ( $\phi$ : uniform)		$\frac{\pi}{4} = .785$	1
direction cosine (Covoyou)	5.42		2
direction cosine (von Neumann)	5.15		2
Compton scattering		.34~.65	3
Compton scattering (improved)		.75~.93	7
pair creation	not shown	not shown	4

Note:

- (1)  $n$  : the number of generated random numbers on the average
- (2)  $p$  : efficiency (reciprocal of  $n$ )
- (3)  $b$  : the number of branches in a program which describes each process .  
The more the number of branches is, the less the PE efficiency is.

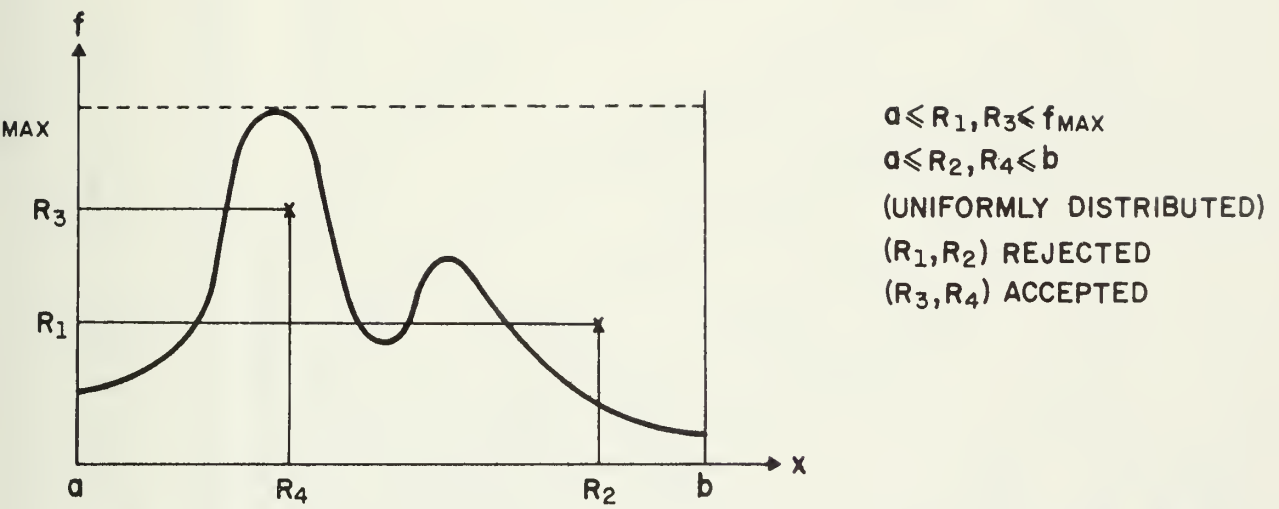


Figure 2.1 The Rejection Method



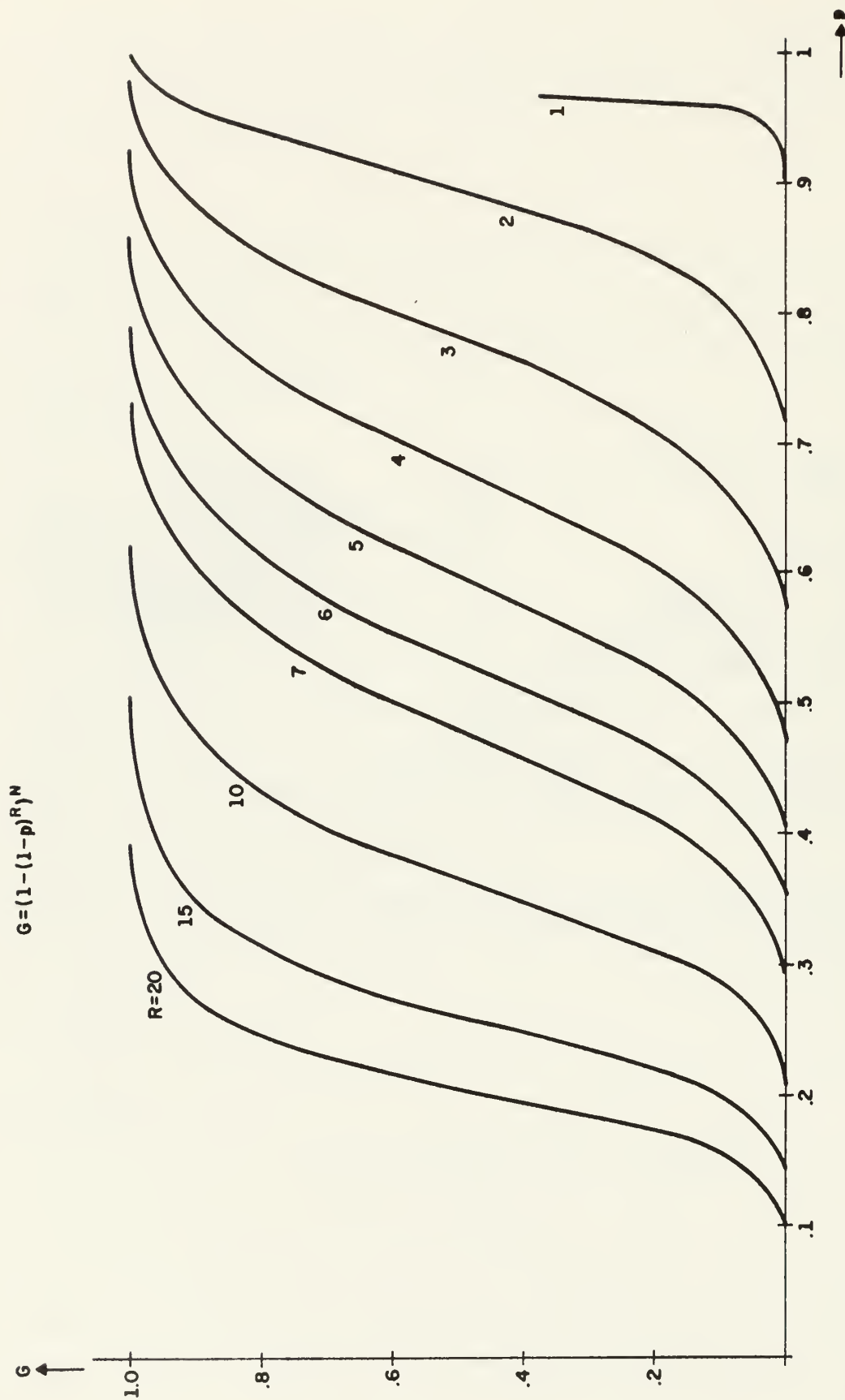


Figure 2.2 Distribution Function of the Probability of Getting All  $N$  Successful Results After  $R$  Trials ( $R$ : parameter,  $N=64$ )



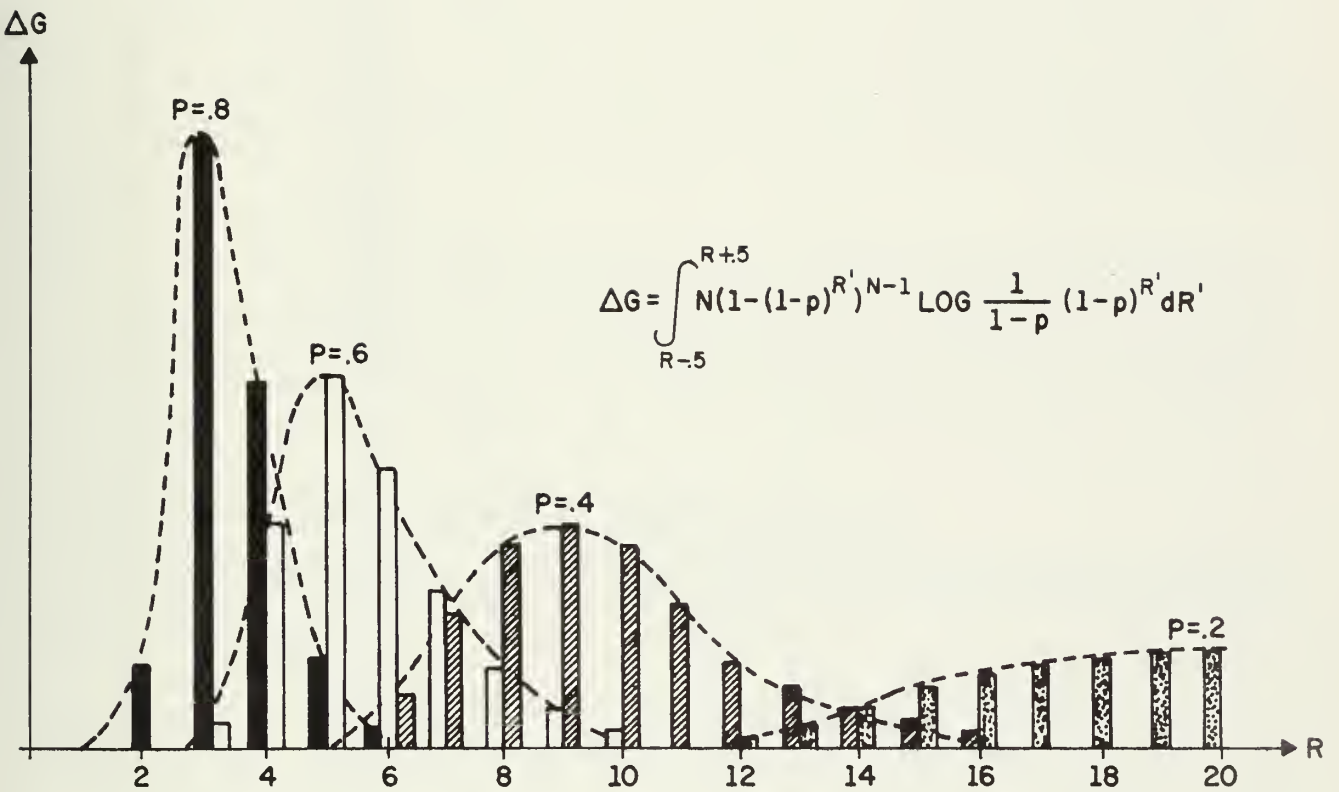


Figure 2.3 The Probability Density Function of the Number of Trials to Get All  $N$  Successful Results ( $p$ : parameter,  $N=64$ )

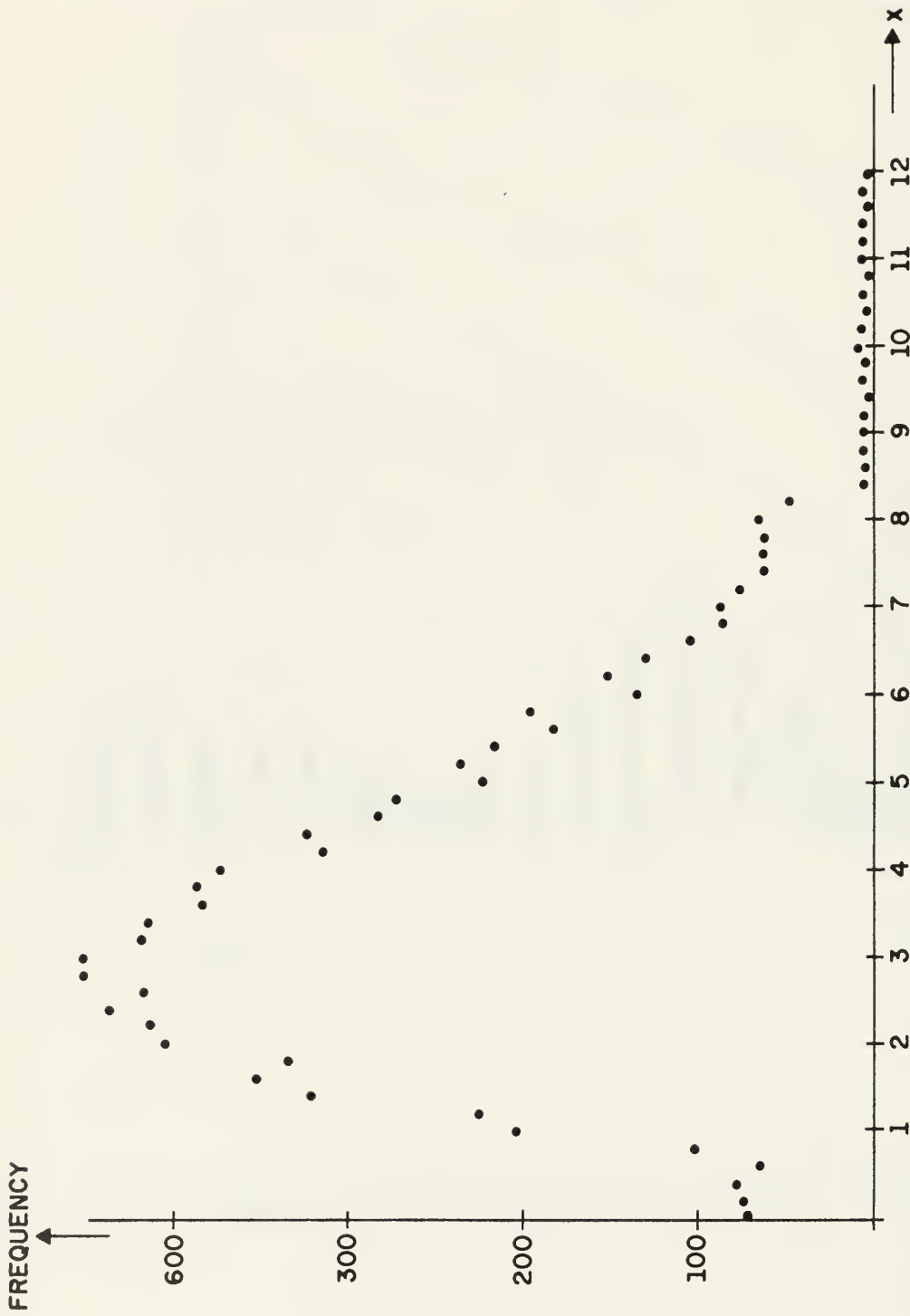


Figure 2.4 An Example of the Method in 2.2.3 Planckian Distribution

$$P(x) = \frac{15}{4\pi} \int_0^x \frac{x^3}{e^x - 1} dx \quad N = 10,000$$

### 3. FUNDAMENTAL STRUCTURE OF THE PROGRAM

Both this chapter and the next chapter describe a parallel version of the Monte Carlo calculation of radiation transport. This chapter is concerned with the fundamental structure and the problem of data storage. In Section 3.1, several basic schemes are discussed and compared. The "Particle Migration Scheme" has been adopted for the problem in Chapter 1.

The actual data structure of the "Particle Migration Scheme" is described in detail in the next section. Several techniques such as conversion of real type data into integers and chain structure are also discussed.

#### 3.1 Basic Program Structures and Their Comparison

##### 3.1.1 Geometrical Structure of the Medium and Hardware Structures of the Computer

It is assumed in the subsequent discussions that the medium is a two dimensional rectangle. Some examples are shown in Figure 3.1. The simplest case is when the density of the medium  $\rho$  is a constant or slow-varying function of coordinates so that the table for  $\rho$  can be contained within a PE. Each PE can then cover the whole domain of the medium. In such a case it does not matter which PE processes which particle; it remains in the same PE until destroyed. The entire program becomes very simple and the efficiency depends chiefly on the number of logical branches.

If the table for  $\rho$  is too large to store in one PE (or too uneconomical), it must be distributed among PEs. In this case, the correspondence of the hardware structure (PEs and their memory) to the geometrical structure of the medium ( $\rho$  table) becomes more explicit. Let the coordinate

system attached to the medium be called the "reference coordinates". As an example, if the X coordinate of the reference corresponds to the location of PE memory and the Y coordinate to PE number then both structures match each other. (Straight storage case) As will be discussed later there are some other ways of storing  $\rho$ 's, in which the correspondence becomes more obscured. As for the particles, there are two different basic points of view which consequently lead to two different program schemes.

The first scheme is to fix the reference coordinates to PEs so that particles are transferred to the neighboring PEs as they move. In other words, each PE is assigned within a certain region of the entire medium. This view is similar to the "Eulerian View" in hydrodynamics and will be called a "Particle Migration Scheme" in the following sections. The second scheme, on the other hand, is that each PE contains a certain number of particles which will be handled in it until they are destroyed. Therefore, the new data on the medium are fetched to a PE in which a particle is stored that requires them. In other words, if one's eyes are fixed on a PE (or the hardware structure) a particle stays in it and the reference coordinates move in to the particle. One confusing thing about this notion is that the motion of the reference coordinates varies with particles. This is to be called the "Coordinate Migration Scheme". The Lagrangean formulation in hydrodynamics is somewhat similar to this scheme. Comparisons of the two schemes will be made in the next sections.

### 3.1.2 Particle Migration Scheme

As has been discussed briefly in the beginning of this chapter, particles actually migrate to the neighboring PE as they cross cell boundaries. This is most efficiently performed by using ROUTE instruction. The merit of this scheme is that the destinations of routing are limited to

very few PEs. This makes a program work very efficiently. (Some statistical results for a simple test program will be discussed in Chapter 5). There are several ways of assigning PEs to the parts of the medium. The simplest one is shown in Figure 3.3-a. In this example, each PE is assigned with a long strip of the domain, i.e., the Y direction corresponds to processor number, whereas the X direction corresponds to the location in the memory of each PE. If the geometrical structure of the material is cylindrical and the source is located at its center, this configuration can be adopted. The advantage is that the routing distances are +1, -1, or 0 so that the program works very efficiently. In the example of Figure 3.3-a, the displacement of particles in the X direction does not involve routing. There is a disadvantage in the straight storage if many particles escape outward from the edge of the medium. Then only PE63 and PEO will have to take care of those which escape in positive and negative y directions respectively after turning off all other PEs. This disparity on the boundary can be solved by skewing the medium as shown in Figure 3.3-b. It is obvious that the boundary is almost equally distributed but there are now 5 different routing distances possible. There is also a problem that the initial allocation of data on density becomes more complicated. (Further comparison of both straight and skewed storage will be discussed in Chapter 5).

If there is no cylindrical symmetry, the best way to distribute the boundary equally is to form 8 x 8 squares (Checkerboard storage). (Fig. 3.3-c,d). In these cases, there are 9 different routing distances each of which corresponds to a neighbor of a cell or a cell itself. If each particle carries a lot of information with it which has to be routed to its destination, the increase in routing deteriorates. The boundary problem

arises in this scheme too. In Figure 3.3-d the boundary is more equally distributed than in Figure 3.3-c.

The conclusion is that the way PEs should be assigned cells is strongly dependent on what type of problem is to be solved and cannot be determined a priori.

Reducing the variables characterizing each particle is as important as reducing the number of different route distances. This will be discussed and illustrated in detail in Section 3.2.

### 3.1.3 Coordinate Migration Method

In contrast to the particle migration method, particles stay in their PEs all through their lives. This method involves a table lookup problem. As time goes on, particles diffuse over the medium. They will require the data on the density stored in various PEs. Generally, this method is not applicable in practical cases. But when the table size describing the density is small enough to store entirely in a few PEs ( $2^4$ ), then the routing distance is limited and this method is usable. The routing procedure for the "reduced density" is simpler than the particle migration method in general, because the number of data to be routed is usually smaller. As this method was not adopted in the program shown in Chapter 4 no further detail will be discussed.

## 3.2 Particle Migration Scheme

### 3.2.1 Particle Tables

Each "particle" in the table consists of such data as cell number, (N), relative coordinates within a cell, (X,Y), direction cosine, ( $\mu$ ), azimuthal angle, ( $\sin \phi$ ,  $\cos \phi$ ), energy, (E), fraction of time interval  $\Delta t$ , ( $\xi$ ), survival distance, ( $\tau$ ), weighting factor, (W), and pointers. All except the last one are physical quantities associated with a particle, which



have been explained in Chapter 1. Pointers, on the other hand, are for higher efficiency of computation. Certain techniques yield less memory requirements and faster computation.

### 3.2.2 Packing Data and Integer-Real Conversion

The memory size problem is very serious because each PE has only 2048 words. Therefore, those previously mentioned data must be packed as densely as possible. Fortunately, GLYPNIR<sup>1</sup> enables any part of a word to be loaded to a register as an integer. If 16 bits are enough for an integer, 4 such data can be packed into a full word. Real numbers, however, can be only full-sized (48 bit mantissa) or half-sized (24 bit mantissa). It is possible to store a real number in the form of an integer if it has some upper limit. Such cases are: direction cosine, azimuthal angle, ( $|\mu|$ ,  $|\sin \phi|$ ,  $|\cos \phi| \leq 1$ ) and relative coordinates ( $0 \leq x, y < 1$ ). To accomplish this, the following rules were used: to store a real number, multiply it by  $2^p$  ( $p = 15$ , for example) and store the obtained integer into some location; to read it out and compute with it, load it to a register as an integer, shift it to the left end of the mantissa part, and change the exponent part. With the combination of these techniques all the data on a particle are packed into 4 full words or less. (Fig. 3.4).

### 3.2.3 Chain Structure

The efficiency of computation is greatly improved by linking particles of the same characteristics (e.g. those to be scattered) to form a chain. The pointers which have been mentioned in the beginning of this chapter are for this purpose. Figure 3.5 shows how a pointer works. If particles of particular interest are not linked, all the particles in the

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1. GLYPNIR is a higher level language for ILLIAC IV. (Ref. [8]).

table must be scanned. (Fig. 3.5-a).

On the other hand a pointer-linked table can be scanned efficiently. Suppose the table size is  $M$ .  $\ell_i$  is the length of the chain in the  $i$ th PE and  $\sigma M$  is the expectation value of  $\ell_i$  ( $i = 0, 1, \dots, 63$ ). Then the number of steps to scan the table is  $L = \max_{0 \leq i \leq 63} \ell_i$

The distinction between the linked and the unlinked is more obvious if the entire table ( $M$ ) consists of several, say  $N$ , subsets and any particle belongs to one of them and only one of them. The number of steps is  $N \times M$  to scan the unlinked table, (because the table must be scanned  $N$  times), while the number of steps to scan the linked table is:

$$L = \sum_{I=1}^N \text{Max}_{0 \leq i \leq 63} (\ell_i(I)) \leq N \times M$$

See appendix 1 for mathematical derivation and an example. An illustrated example is also given in Figure 3.6.

Pointers can be either included in particle tables or separated from them. The first method is good if there are only a few pointers. (Such is the case of the program listed in this paper). But the second method is better if there are many ( $\sim 8$ ) pointers associated with such particles; they need not be routed when a particle crosses cell boundary.

Suppose that every processor contains 100 particles each of which consists of 4 words. The pointer must take values 0, 4, 8 . . . 396 ( $< 512$ ). Therefore, 8 pointers can be packed into a full word (64 bits). (Note that 8 bits are enough for each of them).

### 3.2.4 Material Table

The material table stores data such as energy (temperature), density, specific heat of  $64 \times 32$  cells, besides tables of absorption and scattering coefficients. Each cell is assigned with two full words and data are packed



in the same way as before, some as integers, some as real numbers.

If energy of newly created particles at each time step is to be sampled from a Planckian population, its interpolation table must be stored too.

### 3.2.5 I/O

Because of the limitation of memory size, only a portion of large particle tables can be stored in the PE memories. Therefore, they must be stored in disc memory after being processed sufficiently and a new particle table must be brought into the PE memories. It is not efficient, however, to stop processing while I/O is being done. A better way is to divide each memory into three large blocks titled, NEW, OLD, PROCESS, which corresponds to the area into which a new particle table is being read, the area from which a particle table is stored into disc and the area of currently processed particle tables, respectively. NEW becomes PROCESS, PROCESS becomes OLD, OLD becomes NEW in the next phase and so on. (Fig. 3.7).

### 3.2.6 Total Capacity of Particles

The capacity of particles in the simple case when the medium consists of  $64 \times 32$  cells can be calculated by taking all the above things into consideration:

$$\begin{array}{cc} \text{Particles} & \text{Medium} \\ \underbrace{\hspace{1cm}} & \underbrace{\hspace{1cm}} \\ 3 \times 4 \times N + 32 \times 2 + E & + F \leq 2048 \end{array}$$

where

N : the number of particle table entries

E : table for random sampling (Planckian) + table for absorption and scattering coefficients  $\approx 50$  (non-monochromatic)

0 (monochromatic)

F : instructions and GLYPNIR system  $\approx$  200

$$\therefore N = 1734/12 \doteq 144$$

$$64N \doteq 9200$$

Therefore, about 9200 entries are available for particles.

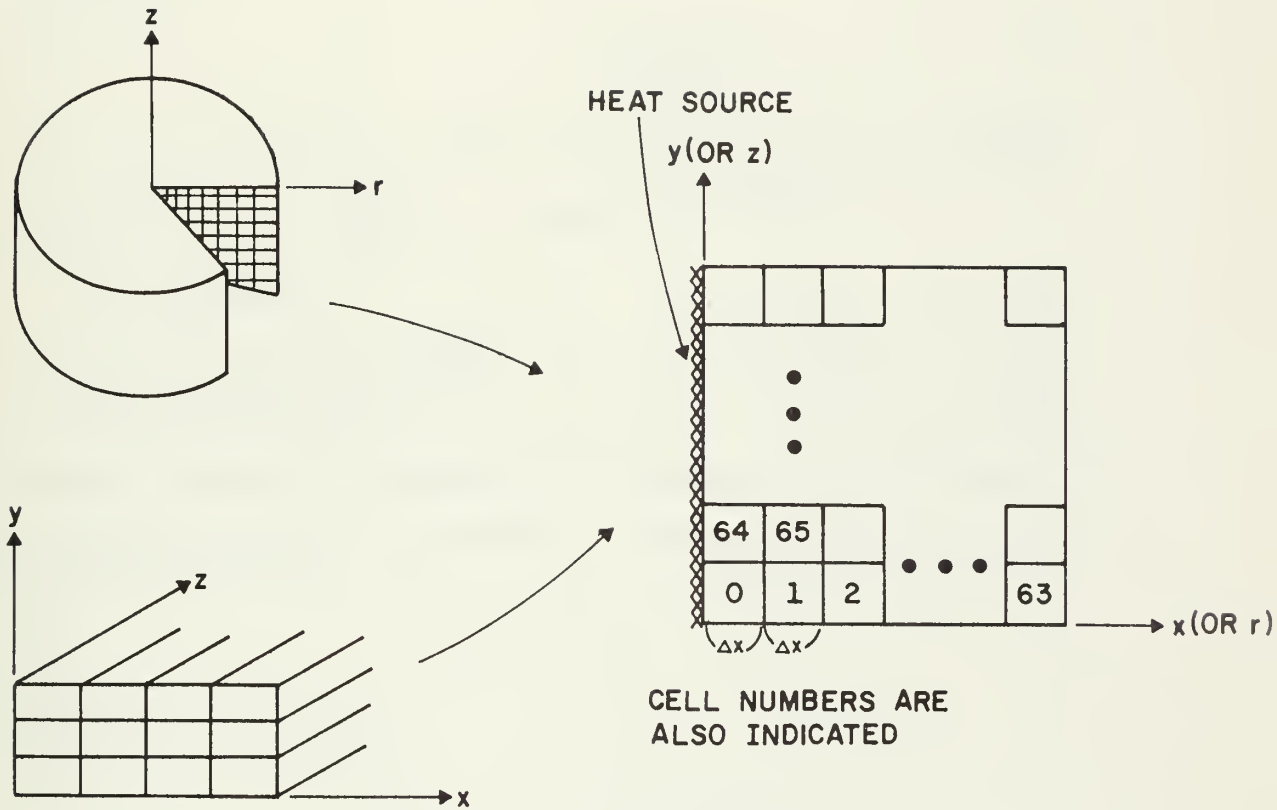


Figure 3.1 Some Examples of Geometrical Structure of the Medium and the Corresponding Cell Number Assignment

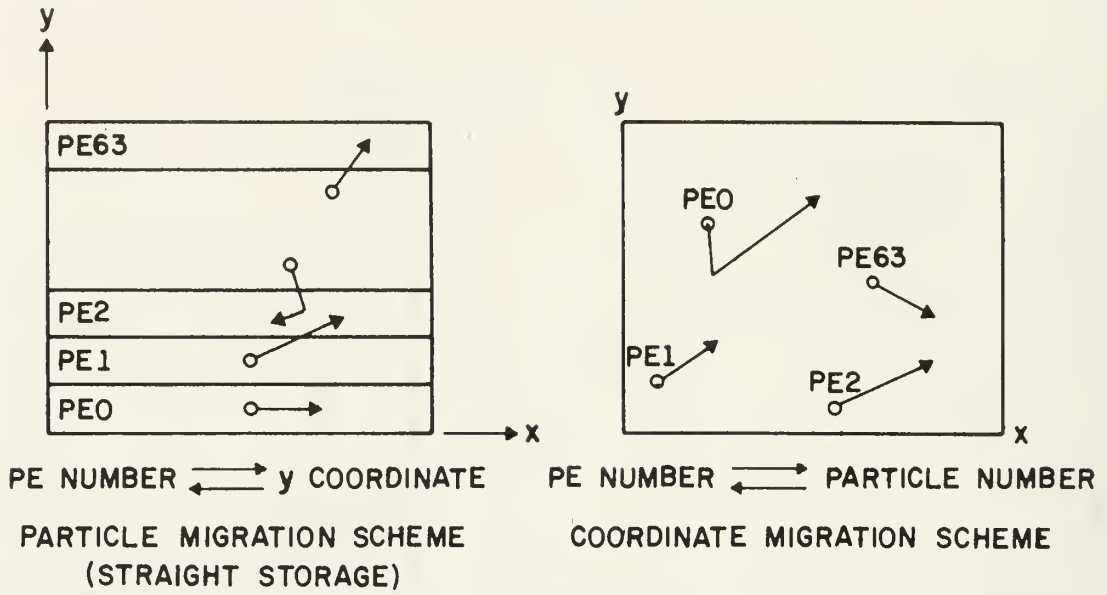
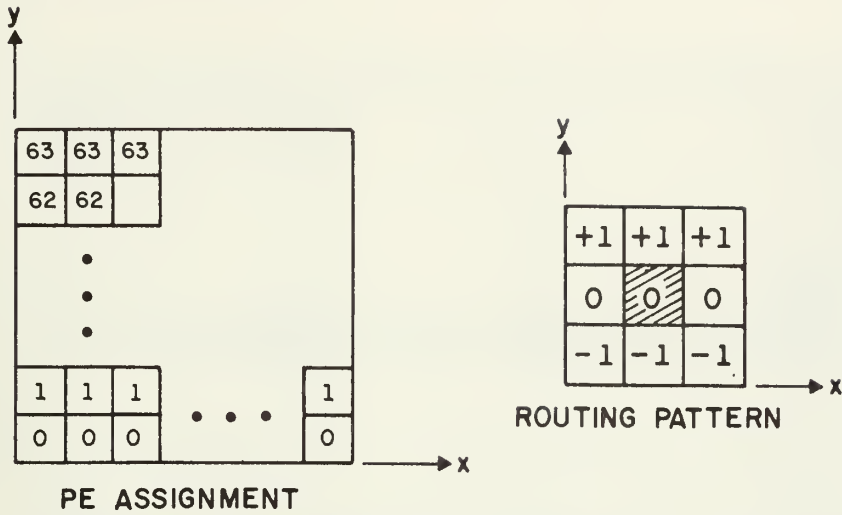


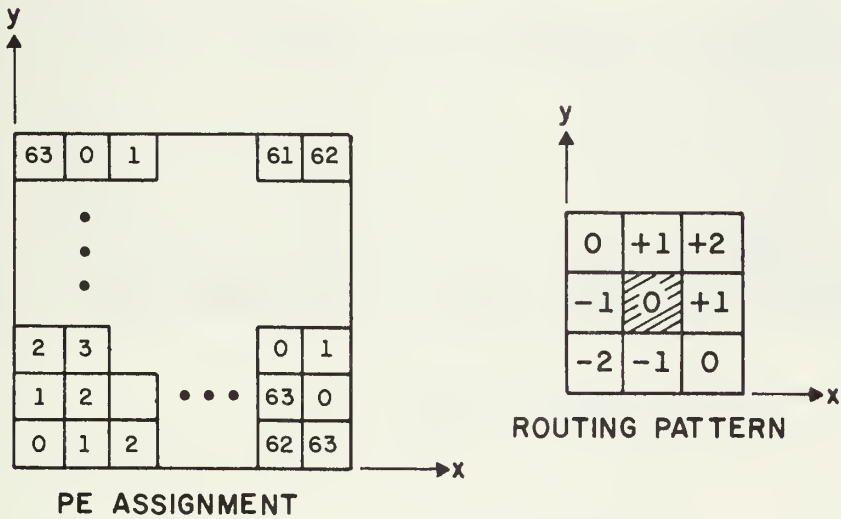
Figure 3.2 Comparison of Two Different Schemes

## (a) STRAIGHT STORAGE



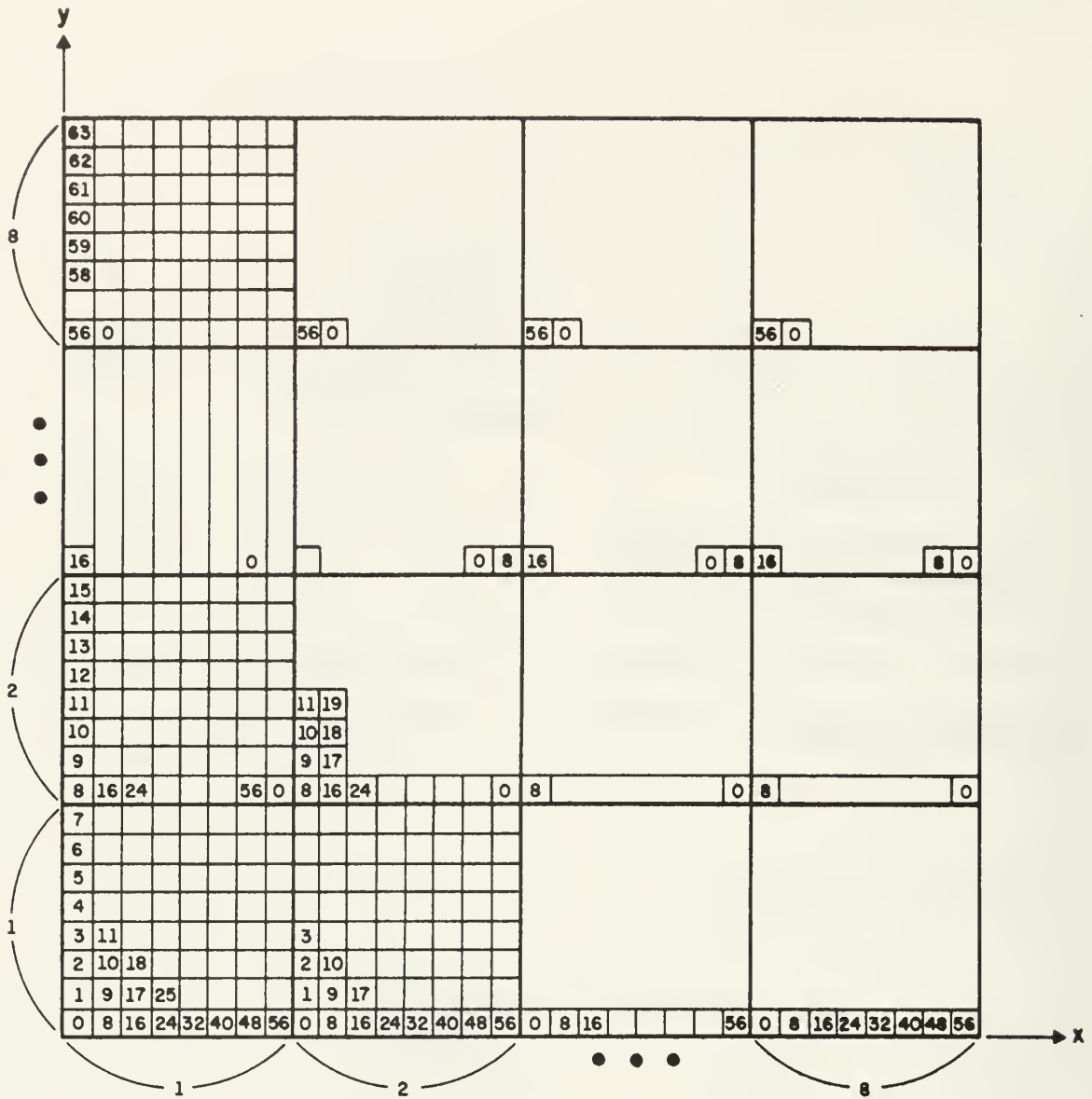
(ALL NUMBERS ARE ASSIGNED  
ACCORDING TO FIG. 3.1)  
PE NO. = CELL NO. DIV 64

## (b) SKEWED STORAGE

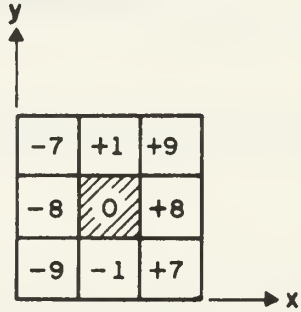


PE NO. = (CELL NO. DIV 64 + CELL NO. MOD 64) MOD 64

Figure 3.3 Some Examples of PE Assignment  
in the Particle Migration Scheme



PE ASSIGNMENT (64 x 64)



ROUTE PATTERN

Figure 3.3-c Some Examples of PE Assignment in the Particle Migration Scheme (continued) - Straight Checkerboard Storage

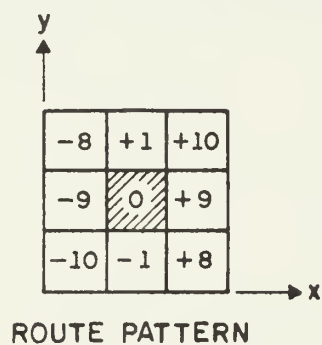
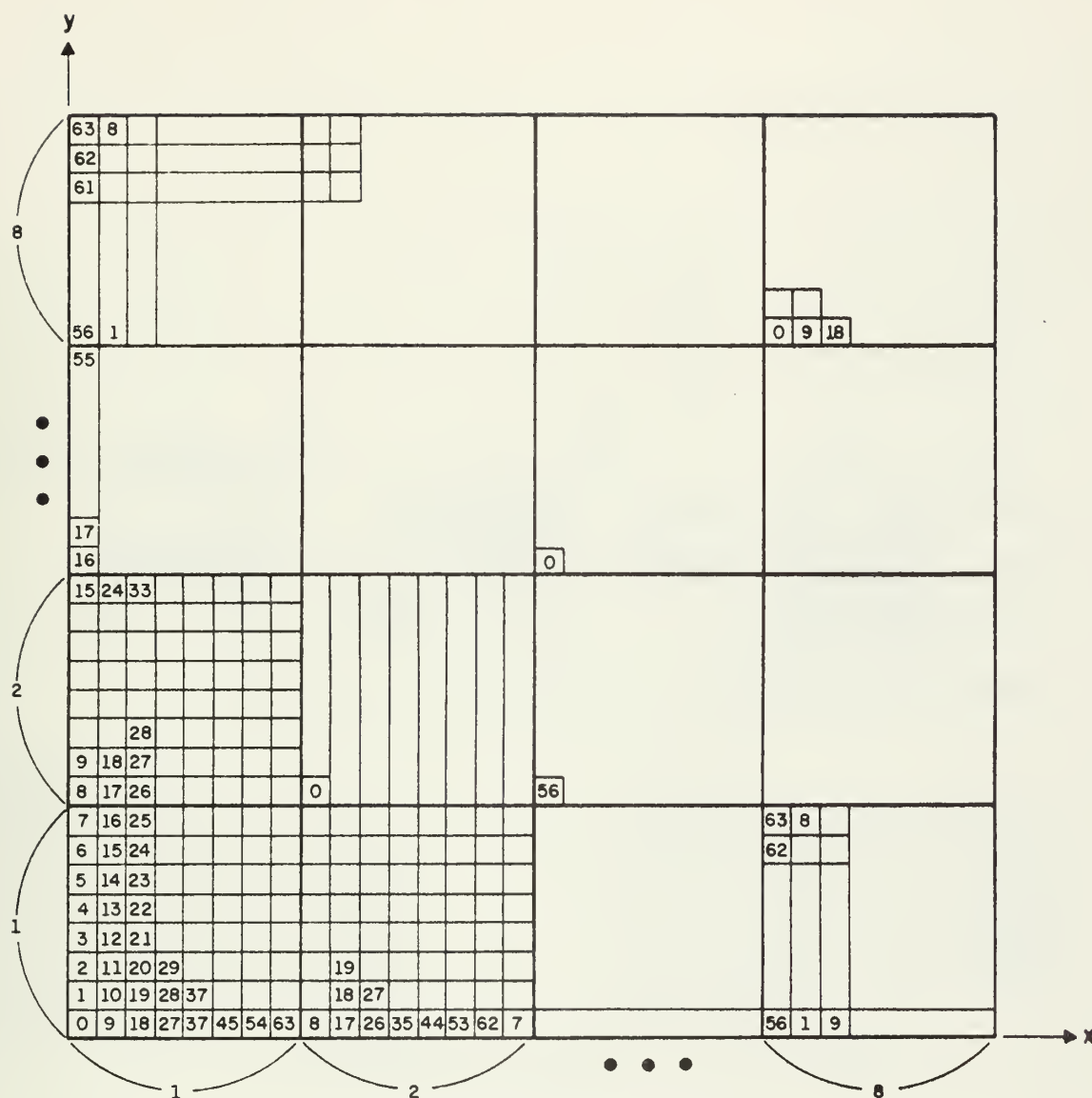


Figure 3.3-d Some Examples of PE Assignment in the Particle Migration Scheme (continued) - Skewed Checkerboard Storage

TNB+0	CELL NO.	POINTER 1	x	y
TNB+1	SIN $\phi$	POINTER 2	$\mu$	COS $\phi$
TNB+2	$\xi \Delta t$		ENERGY	
TNB+3	WEIGHT		$\tau$	

Figure 3.4 An Example of Particle Table  
(used in the test program in Appendix 3)



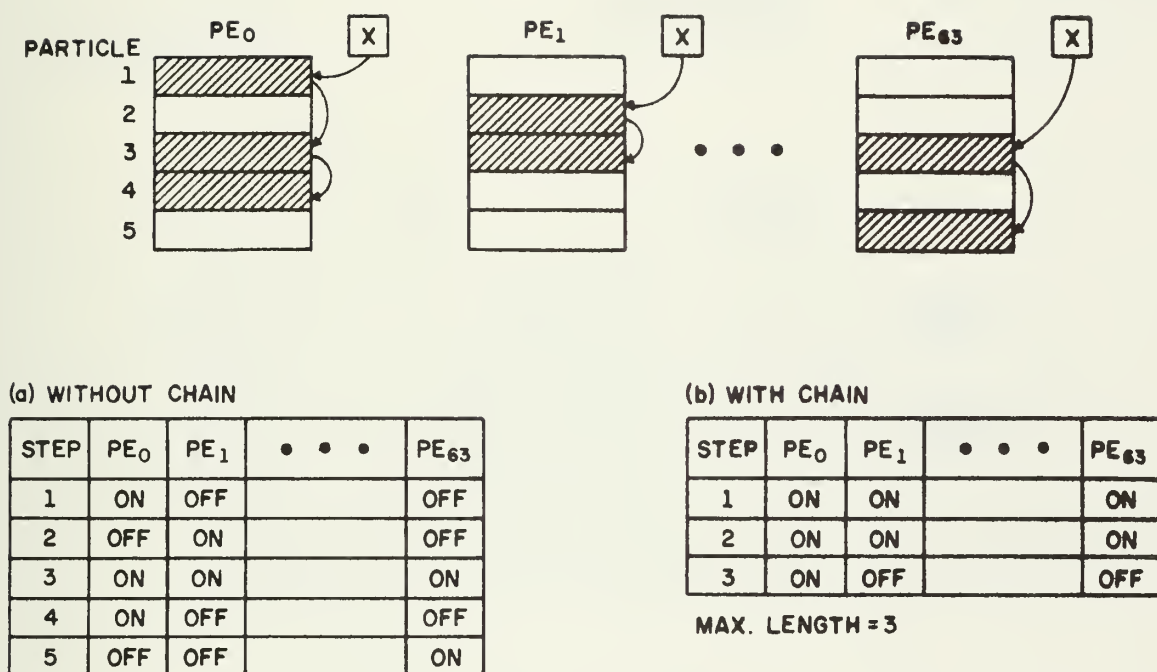
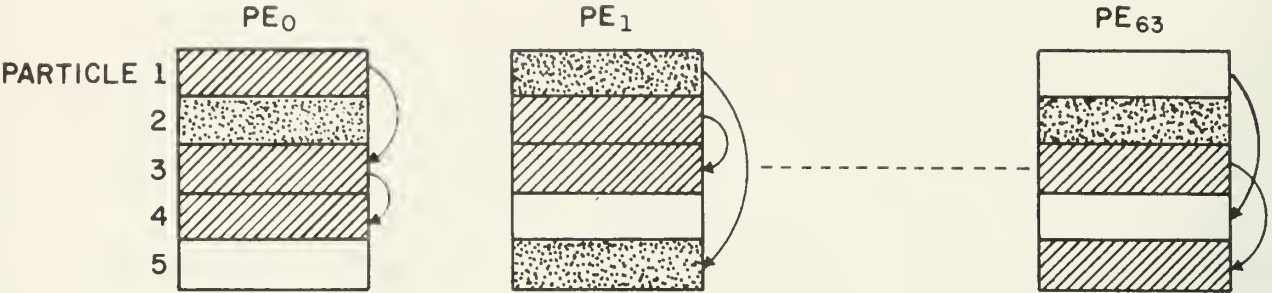


Figure 3.5 Comparison of a Chain-linked Table and a Usual Table






TYPE	NO. OF STEPS	PE			
	1	#1	#2	-----	#3
	2	#3	#3	-----	#5
	3	#4	OFF	-----	OFF
	4	#2	#1	-----	#2
	5	OFF	#5	-----	OFF
	6	#5	#4	-----	#1
	7	OFF	OFF	-----	#3

Figure 3.6 Another Example of Chain-linked Table

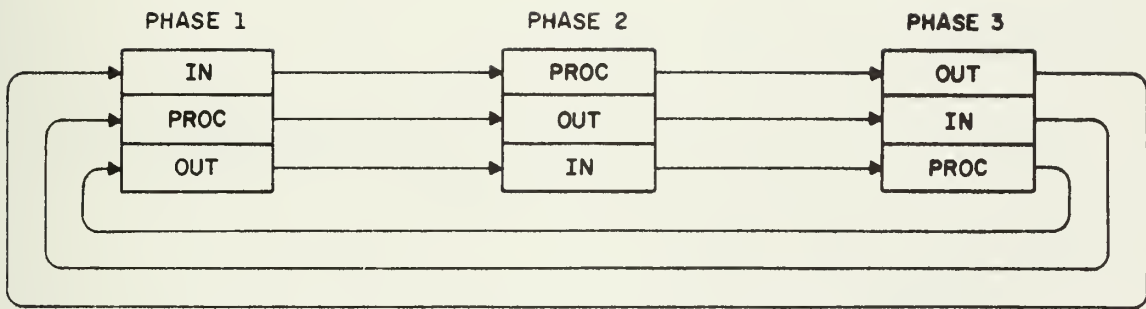


Figure 3.7 Three Phases in I/O

#### 4. A TEST PROGRAM FOR ILLIAC IV

This chapter is concerned with the description of the program which was written in GLYPNIR (Ref. [8]) and was run on simulator SSK. (Ref. [17]). It is given in Appendix 3. This program was written to test the feasibility of parallel computation for this problem and also to serve as an example for more detailed programs.

The simplifications which were made for this test program were discussed in Section 1.3. A flow chart is in Figure 4.1.

The whole program consists of about 20 small subroutines, names of which are given in Table 4.1.

##### 4.1 Description of Major Subroutines

DATALOAD--All the numerical quantities which are necessary to initialize the programs are read in. These are:

- (1) initial random numbers
- (2) the length of one time step ( $\Delta t$ )
- (3) mass absorption coefficient ( $\sigma_{\text{abs}}$ )
- (4) mass scattering coefficient ( $\sigma_{\text{scatt}}$ )
- (5) density distribution
- (6) specific heat distribution
- (7) initial temperature distribution

CHAIN--This subroutine is to link the table entries of some common characteristics (such as scattering, routing, etc.) to form a chain. It was briefly mentioned in Chapter 3. It functions as follows: Suppose the Nth table entry is to be linked to the chain for scattering. First, the pointer part of the Nth entry is replaced by the contents of a register which always keeps the location of the edge of the

chain for scattering. Then N (which is the most up-to-date location of the edge) is stored into the register.

Due to the necessity for handling two different pointers by one subroutine, indexing facility is also included. Namely, either of two pointer parts of a particle table entry can be specified by changing an input parameter Q.  $Q = 0$  for scattering and vacancy, whereas  $Q = 1$  for routing.

CVTRL--This subroutine divides a 15 bit integer by  $2^{15}$  without using division. It was also discussed in Chapter 3.

RNDX--This is a random number generator which generates uniformly distributed random numbers by the linear congruential method. See Chapter 2 for detail. Initial random numbers are read into PEs at the beginning of the program.

ENERGYBALANCE--This subroutine calculates the energy to be emitted by radiation in each cell. The total radiative energy is summed up to assign the number of particles in the next subroutine.

PARTICLEASSIGN--The number of new particles in each cell of the medium is determined. It is proportional to the radiative energy in the cell. To avoid the overflow problem of particle table, only the two-thirds of the available vacancy in PE is used to create new particles. The energy per "particle" is merely (the radiative energy per cell)/(the number of particles in the cell). That is, the energy is monochromatic.

The whole program has been made so that the radiation process can be extended in the future to non-monochromatic case. The weighting factor in the particle table, for example, is meant for this purpose. If the radiation is not monochromatic, tables for absorption and scattering coefficients as well as data for Planckian distribution must be

stored in PE memory.

BIRTH--New particles are created in this subroutine according to Section 1.3.

TRANSLATE--This subroutine has two functions. One is to translate particles to their new locations. The other is to detect those particles which cross the cell boundaries and those which escape from the medium.

ABSORB--This subroutine is called when a particle is absorbed by the medium. The particle is destroyed and its table entry is linked to the VACANCY chain.

ESCAPE--This subroutine is called when a particle escapes from the medium. The particle is also destroyed, its table entry is linked to the VACANCY chain, and ESCAPE counter is incremented by its weight.

BRANCH--This subroutine calls TRANSLATE, decides interaction types of particles, then calls ABSORB, ESCAPE to process particles. Those which are to be scattered are not processed here but linked to form a chain. This is because the scattering process is very long and it is desirable to process them in parallel at a later time. Those particles which cross the cell boundaries toward the y-direction are also linked for routing. This subroutine is called both in the main program and SCATTER.

ANGLE--New sets of angles after Thomson scattering are calculated. The algorithm to sample the scattering angles was described in Section 2.2. New angles are then obtained by using spherical trigonometric formulae in Section 1.1.

SCATTER--Particles in the chain for scattering are processed after the table scanning is finished in the main program. This subroutine

calls ANGLE, BRANCH, STORE, and functions almost in the same way as the main program does to scan the table.

ROUTE--Particles in the chains for routing are actually transferred to their destinations in this subroutine. Index  $K = 1$  specifies the routing to the right and  $K = -1$  specifies the routing to the left. The vacancy which has just been made is linked to the VACANCY chain.

TALLY--This subroutine is used to sum up the intensity of radiation in each cell. The summed intensity is necessary in ENERGYBALANCE to calculate the new temperature.

#### 4.2 Main Program

The main program contains all the global variable and subroutines and calls the subroutines in the sequence given in Figure 4.1.

The main program starts with the reservation of blocks for PCPOINTERS. The constants and counters are initialized. All the particle table entries are linked as vacancy. A large loop for iterations is entered, one step of which corresponds to the time interval  $\Delta t$ . The radiative energy computed in ENERGYBALANCE decides the particle distribution in PARTICLEASSIGN. BIRTH follows it to create new particles in the vacancy. Then the table scanning starts, (this is a sequential scanning from the top to the bottom), during which the coordinates of particles are updated, the types of interactions are determined, and so on. After all the entries of the particle table are scanned, the main program proceeds to the scattering process SCATTER, which is followed by ROUTE and TALLY. This completes one time cycle and the intermediate results may be printed out by TABLEPRNT. The entire program consists of more than 800 cards in source code (including comment cards) and is compiled into more than 5,500 instruction syllables



of assembly codes. About 220 words of PE memory in every PE are occupied by these instructions.

Table 4.1

Name	Function	Type	Called By
ABSORB	Absorption		BRANCH
ANGLE	New Scattering Angles		SCATTER
BIRTH	Creat New Particles		MAIN
BRANCH	Interaction Type		MAIN
CHAIN	Table Link		PARTICLEASSIGN, BIRTH, BRANCH, SCATTER, TRANS- LATE, MAIN
COS	Cosine	PREAL	BRANCH
CVTRL	Integer→Real	PREAL	BRANCH
DATALOAD	Initial Data		MAIN
DSTBND	Distance to Boundary		BRANCH
ESCAPE	Count the Number of Escapes		BRANCH
ENERGYBALANCE	New Energy		MAIN
EXP	Exponential	PREAL	
LN	Natural Log	PREAL	BIRTH, SCATTER
MOD	Mod (64)	PINT	BIRTH, TRANS LATE
PARTICLEASSIGN	Number of Particles to be Created		MAIN
RNDX	Random Number	PREAL	BIRTH, ANGLE
ROUTE	Routing to Neighbors		MAIN
SCATTER	Scattering		MAIN
SIN	Sine	PREAL	BIRTH, ANGLE



Table 4.1 (con't)

Name	Function	Type	Called By
SQRT	Square Root	PREAL	BIRTH, ANGLE
STORE	Store to Particle Table		MAIN, SCATTER
TABLEPRNT	Print out the Contents of Tables		MAIN
TALLY	Intensity of Radiation in each Cell		MAIN

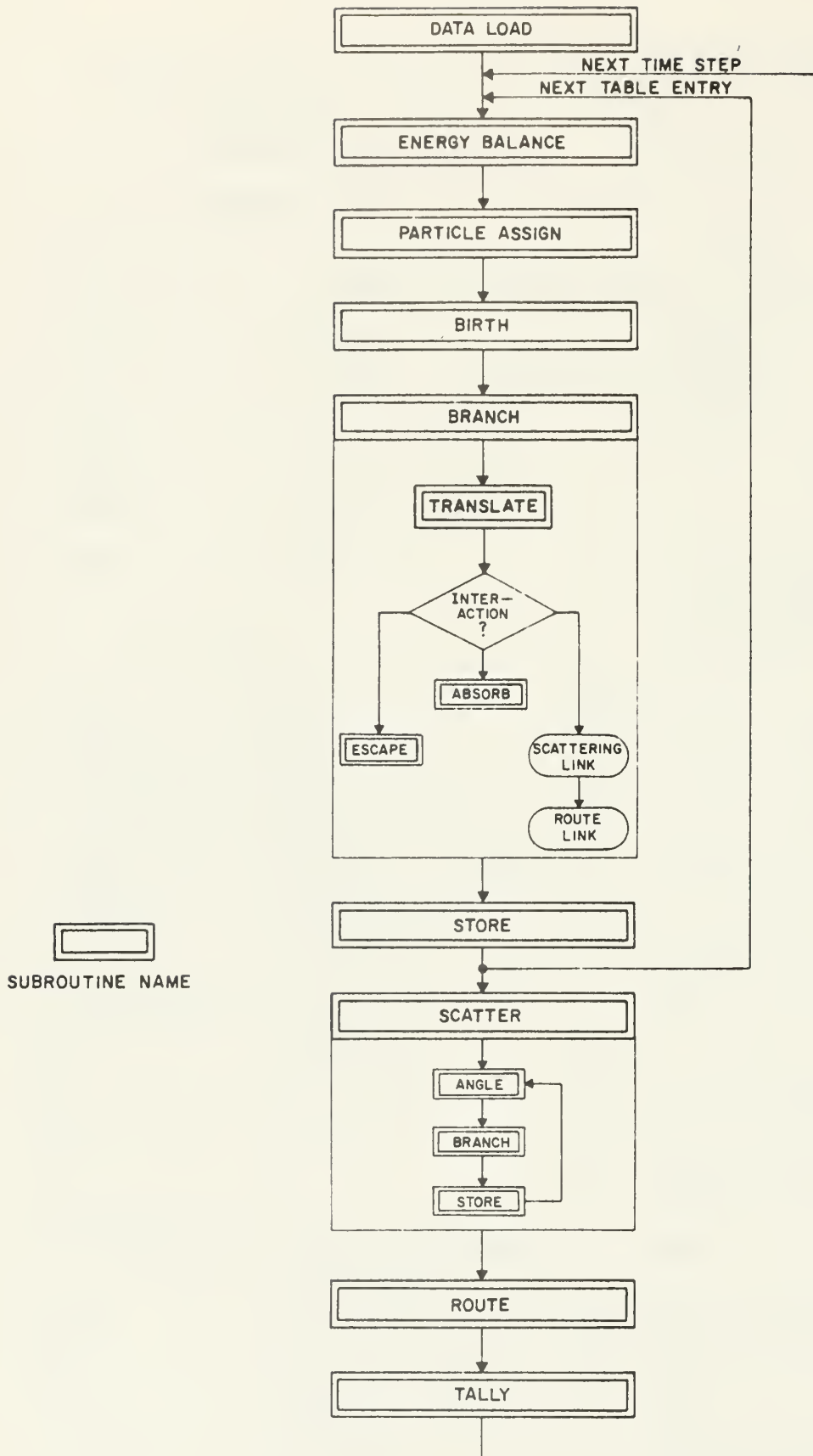


Figure 4.1 A Flow Chart of the Test Program

## 5. SOME COMPUTATIONAL RESULTS

Some of the computational results are discussed in this chapter. Since the simulator works very slowly, it is not practical at the present time to run the whole program for many time steps. Therefore, ~~emphasis~~ was put on the statistical investigation of PE efficiency aspects. Some factors investigated here are:

- (1) cell size vs velocity
- (2) effect of multiple scattering
- (3) effect caused by using modified probability density function for the survival distance ( $\tau$ )
- (4) effect of skewed storage

All the test programs have been run under the following assumptions:

- (1) the material is homogeneous
- (2) no absorption is involved
- (3) scattering cross section is a constant ( $\sigma$ )
- (4) scattering is isotropic
- (5) mesh size is  $64 \times 8$  except one case ( $64 \times 64$ )

### 5.1 Determination of Cell Size ( $\Delta X$ ) and Time Interval ( $\Delta t$ ) and Their Relation to the Rate of Boundary-Crossing

It is important to know how many particles involve routing. This rate is predicted to be dependent on  $v\Delta t/\Delta X$ . Figure 5.1 shows some computational results. Sixteen particles are created in each PE at the beginning of the time interval  $\Delta t$ . Scattering cross section is taken as a parameter. The rate grows quite linearly with  $v\Delta t/\Delta X$ . This means that  $v\Delta t/\Delta X$  does not affect the efficiency as far as routing is concerned; if  $\Delta t$  is doubled then the number of time steps is halved. The rate decreases somewhat with the

increase of  $\sigma$  because some of the particles which have crossed boundaries are scattered back to their original cells.

The cell size  $\Delta X$  must be determined uniquely by how the density ( $\rho$ ) of the medium varies with position. If  $\rho$  changes very slowly, each PE can cover a wider range (i.e., large  $\Delta X$ ) and vice versa.

$\Delta t$  has an upper limit; no particle can travel through two or more cells in one time step, i.e.,  $v\Delta t \leq \Delta X$ . Within this limit,  $\Delta t$  can be chosen arbitrarily. Small  $\Delta t$  will bring more accurate results on the temperature and the intensity, but the number of time steps increases. Large  $\Delta t$ , on the other hand, will bring more crude results in shorter time. In this case, more routing is involved in each time step. Refer to Section 5.5.4 for a related topic.

## 5.2 Effect of Multiple Scattering

If a particle experiences more than one scattering in  $\Delta t$ , the efficiency of parallelism obviously decreases. Therefore, it is important to see the relation of multiple scattering to scattering cross section  $\sigma$  and  $\ell = V\Delta t$ . The process is simply a Poisson process if  $\sigma$  is constant. Therefore, the probability that a particle is scattered  $n$  times while it travels the distance  $\ell$  is:  $P_n(\ell) = \frac{(\sigma\ell)^n}{n!} e^{-\sigma\ell}$ . (Derivation is in Appendix 2). Figure 5.2 shows the theoretical curve (solid lines) and the result of computation. It is obvious that the number of multiple scattering increases with  $\ell$ . At  $\ell=1$  about 20% of the particles are scattered twice or more. Multiple scattering is treated just as usual scattering in the program described in Chapter 4: if a particle is re-scattered after a scattering, then it is linked again to the top of "scatter chain". Therefore, it is processed together with some others which are located in different PEs and are to be scattered for the first time.

It is not a good idea to enable PEs for only the second scattering after each scattering, then to switch to the third and so on. . . . Statistical fluctuation would work in the most unfavorable way.

### 5.3 An Effect Caused by Modifying a Probability Distribution Function for Survival Distances of Particles

An effort was also made to modify the probability density function for survival distance to reduce the rate of multiple scattering. One method is simply to cut off the density function below some value  $\ell=a$ . This results in shifting all  $P_n(x)$ s ( $n \geq 1$ ) to the right by  $a$  with the exception that  $P_0(x)=1$  ( $x \geq a$ ). If  $a$  is chosen to be  $v\Delta t$ , then there will be no multiscattering at all. But this is too unnatural. The second method investigated gives a linear growth up to  $x=a$  and exponential decay. (Fig. 5.3).

Starting at  $x=0$ , each curve seems to be located between the one sampled from  $P(\tau)=e^{-\tau}$  and the one from  $P(\tau)=e^{-(\tau-a)}$ , but it soon exceeds the former. There is an unusual increase due to the sharp peak in the function  $P(\tau)$  at  $x=a$ . For smaller  $x$ , however, the rate of scattering is reduced. Some order of the Erlang distribution will give a smoother result.

### 5.4 Skewed Cell Boundaries Vs Straight Cell Boundaries

It was stated in Chapter 3 that the skewed cell boundaries smooth out the distribution of the number of particles which escape from the medium. The ideal case is when the mesh size of the medium is  $64 \times 64$ ; every PE has the same number of edges. (Fig. 3.3-b). This scheme, however, increases routing. Therefore, it is necessary to check which method is better. Several tests have been made to compare these two schemes.

The mesh sizes for testing were  $64 \times 8$  and  $64 \times 64$ ; in each case the same data were interpreted in two ways; skewed case and straight case. Results are shown in Table 5.1 and Figures 5.4, 5.5. The conditions

for numerical experiments are the same as before: isotropic scattering, constant  $\sigma$ , and each particle travels for the time  $\Delta t$ .  $\Delta x=1$ .  $\sigma$  and velocity are specified in each case.

#### 5.4.1 64 x 8 Cells

Data were taken for  $\sigma=.4$ , velocity=1, and  $\sigma=.2$ , velocity=.5.

Ten particles were created in each cell at the beginning of a time step and they were all destroyed at the end of this time step. This process was repeated 5 times and the contents of the counters were accumulated. Therefore, effectively 40 particles were examined in each cell (not in each PE). Unnecessary subroutines were removed. In Figures 3.3-a and 3.3-c, there is a peak which is due to the PEs corresponding to the edges of the medium. These peaks were fairly smoothed out in the skewed cases shown in Figures 3.3-b and 3.3-d. As for routing, the distributions turned out to be Gaussian-like in all examples. Obviously, more routing is involved in the skewed storage. Also shown are the distributions of the double routing in skewed storage. That is, the number of particles which have to be routed twice to get to their destinations. (Fig. 3.3-a).

Table 5.1 is the summary of these numerical experiments. The numbers "max-min" in the first column of each experiment mean the maximum and minimum numbers of particles among PEs, respectively, which escaped from the medium or crossed the cell boundaries. "PE average %" means the average percentage of enabled PEs. This was obtained from:

$$\text{PE average \%} = \frac{\sum_{\text{PE}=0}^{63} (\text{counter (PE)})}{\text{max} \times 64} .$$

For example, (49-4, 24%) in the first row means that there were 49 particles escaped from one PE whereas there were only 4 particles from another PE.

All others are between these two values. Therefore, 49 steps are taken to

process these particles in parallel, and 24% of PEs are enabled on the average.

#### 5.4.2 64 x 64 Cells

Data were taken for  $\sigma=.4$ , velocity=1, and  $\sigma=.2$ , velocity=.5. Only the first example is shown in Figure 5.5. Only one particle was created in each cell at the beginning of a time step and they were destroyed at the end of this time step. This process was repeated 5 times so that 5 particles were examined in each cell effectively. Obviously the number of escapes is smoothed out across PEs. The lower half of Table 5.1 can be read in the same way as described in Section 5.4.1. The conclusion is that the skewing does not always bring more favorable results than the ordinary storage.

It is true that the particles that escape from the medium are very well distributed across PEs, but the increase of the number of routing is so big that it cancels out this merit. Therefore, the skewing is better than the ordinary storage only in limited cases such as when ESCAPE takes a much longer time than ROUTE.

### 5.5 Concluding Remarks

The program which is described in this document is a very simple one and expandable to more complicated cases. It is inevitable, however, that the efficiency goes down as the program becomes more complicated.

There are several problems which are left to be solved.

#### 5.5.1 Problem of Table-Overflow and Normalization

As was discussed in Chapter 3, the particle migration scheme has been adopted to obtain higher efficiency in parallel computation. As a consequence, however, particles must be physically transferred to other PEs. If many particles flow into one PE, it will not be able to accept all of them. To encounter this problem, certain number of table entries must be



saved in PEs for those visitors.

Cells must be well distributed among PEs so that the outgoing particles cancel the incoming particles on the average; if many particles flowed into one PE, it would not be able to accept all of the particles. This is an extreme case, but a certain number of table entries still must be saved in PEs as buffers for those visitors. There is a technique called "Russian Roulette" in which incoming particles are rejected with probability  $p$  and accepted with the probability  $1-p$ . In the latter case, the weighting factors are multiplied by  $1/(1-p)$ . This is one of the typical techniques to reduce variances. Special care must be taken, however, when it is used.

#### 5.5.2 Problem of Word Size (alternative format)

When the program was originally implemented, an emphasis was put on the capacity of the particle table. Consequently, only 16 bits were assigned to those words which range in  $[-1,1]$ . But if more accuracy is needed on those quantities, three of them can be packed into one full word. In this case, each word has 21 bits, which is comparable to the fraction part of a half-word (24 bits). An example of word format is given in Figure 5.6.

#### 5.5.3 About the Flexibility of Logical Network Which Interconnects PEs

In the problems which involve probabilistic nature, it is highly desirable that the interconnection of PEs be as flexible as possible. A good example is the table look up problem which was discussed in Chapter 2. If the interconnection logic is programmable by users it will be much easier to handle more complicated problems. This may be one way parallel computers should be organized.

#### 5.5.4 Variable Contraction Ratio of Cell Sizes

It is possible to change the cell sizes in X direction, Y direction, or both. Take Y direction, for example. If the density gradient is not



uniform in Y direction, it is better to adjust  $\Delta Y$  so that it covers a wider range when the density varies slowly and a narrower range when the density varies rapidly in that direction. The reduction ratio,  $\alpha_i$ , in each row of cells is stored as a PE variable and the displacement of particles in Y direction is modified as

$$Y \leftarrow Y + \alpha_i V \Delta t \sqrt{1-\mu^2} \cdot \sin \phi$$

when the particles are in the  $i$ th row of cells.

Survival distance and the displacement in X direction are not changed in this example.

Table 5.1

		$\sigma v$	$\sigma = .1, v = .5$		$\sigma = .4, v = 1$	
			Max. - Min.	PE average %	Max. - Min.	PE average %
64x8	S T R A I G H T	Escape	49 - 4	24%	90 - 9	23%
		R. Route	53 - 0	72%	94 - 0	73%
		L. Route	52 - 0	72%	91 - 0	78%
	S K E W	Escape	26 - 5	53%	45 - 9	46%
		R. Route	69 - 44	85%	103 - 59	80%
		R. Db1. Route	9 - 0		22 - 6	
		L. Route	70 - 43	84%	103 - 58	82%
		L. Db1. Route	8 - 0		21 - 7	
64x64	S T R A I G H T	Escape	35 - 0	5.7%	62 - 0	6%
		R. Route	53 - 26	71%	85 - 50	75%
		L. Route	50 - 27	74%	89 - 52	74%
	S K E W	Escape	5 - 0	40%	10 - 0	44%
		R. Route	82 - 46	74%	93 - 65	85%
		R. Db1. Route	10 - 0		23 - 4	
		L. Route	76 - 36	83%	104 - 60	79%
		L. Db1. Route	9 - 0		22 - 6	

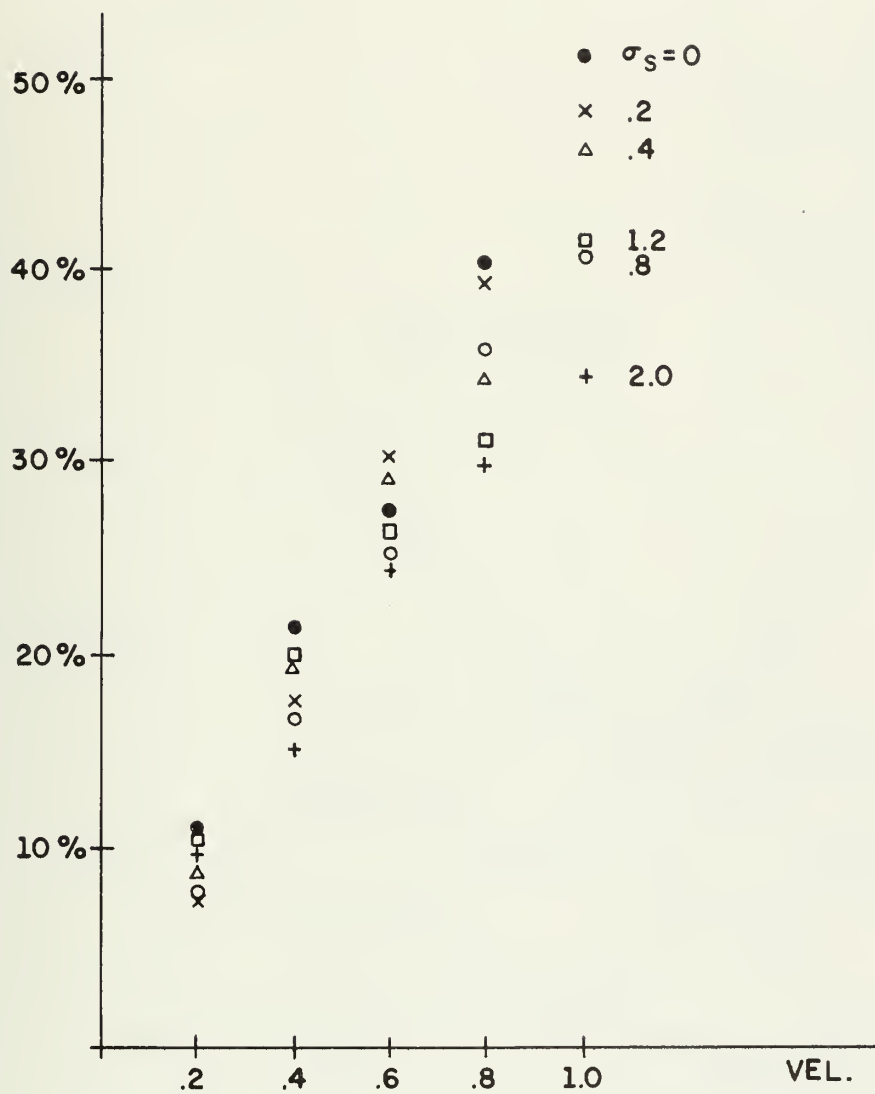


Figure 5.1 Percentage of Particles Which  
Have Crossed Cell Boundaries Vs Velocity  
s: parameter (isotropic scattering)  
 $\Delta x=1, \Delta t=1$  1024 particles

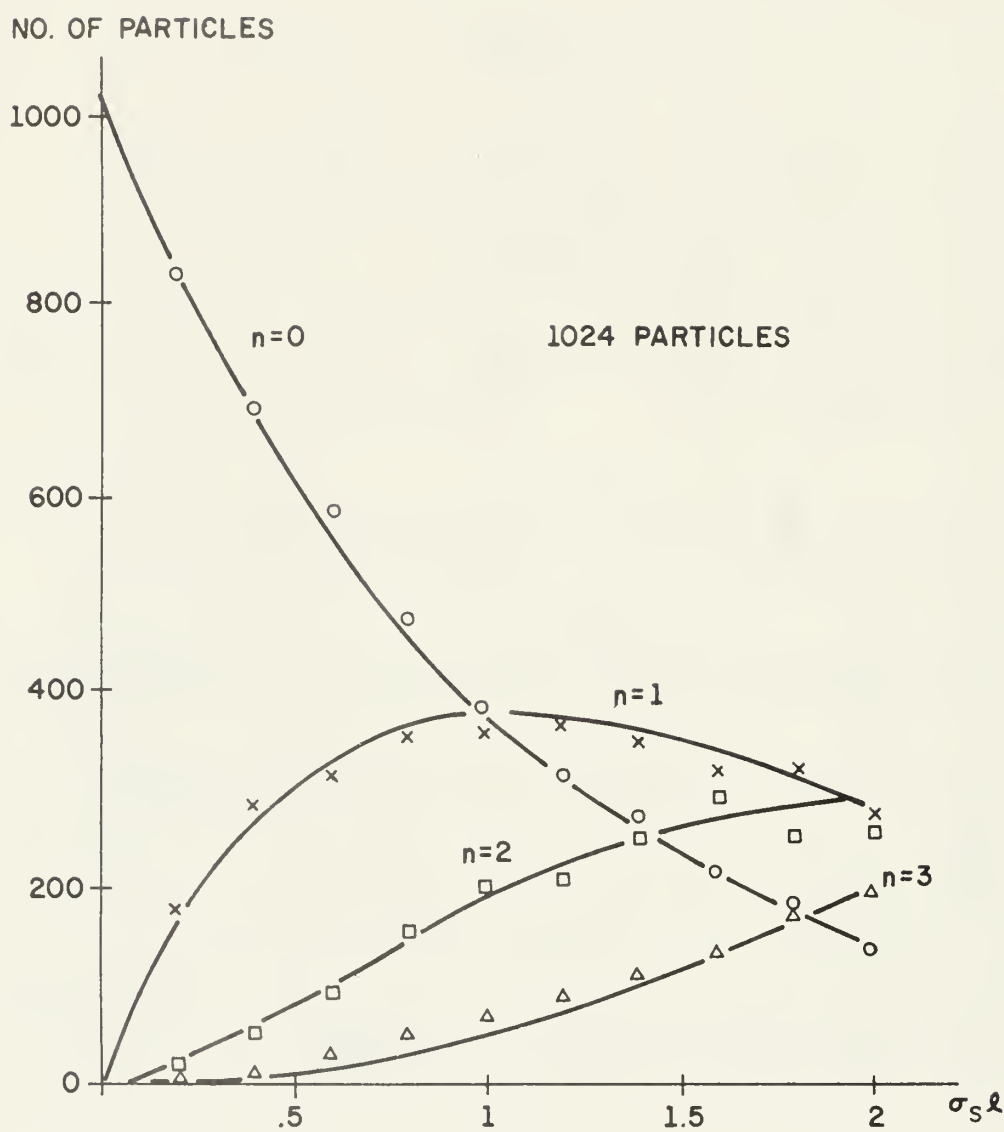


Figure 5.2 Multiple Scattering During  $\Delta t=1$  vs  $\sigma_s \ell = \sigma_s v \Delta t$  (isotropic scattering)  
 (Solid curves are  $P_n(\ell) = \frac{(\sigma_s \ell)^n}{n!} e^{-\sigma_s \ell}$   $n=0,1,2,3$ )

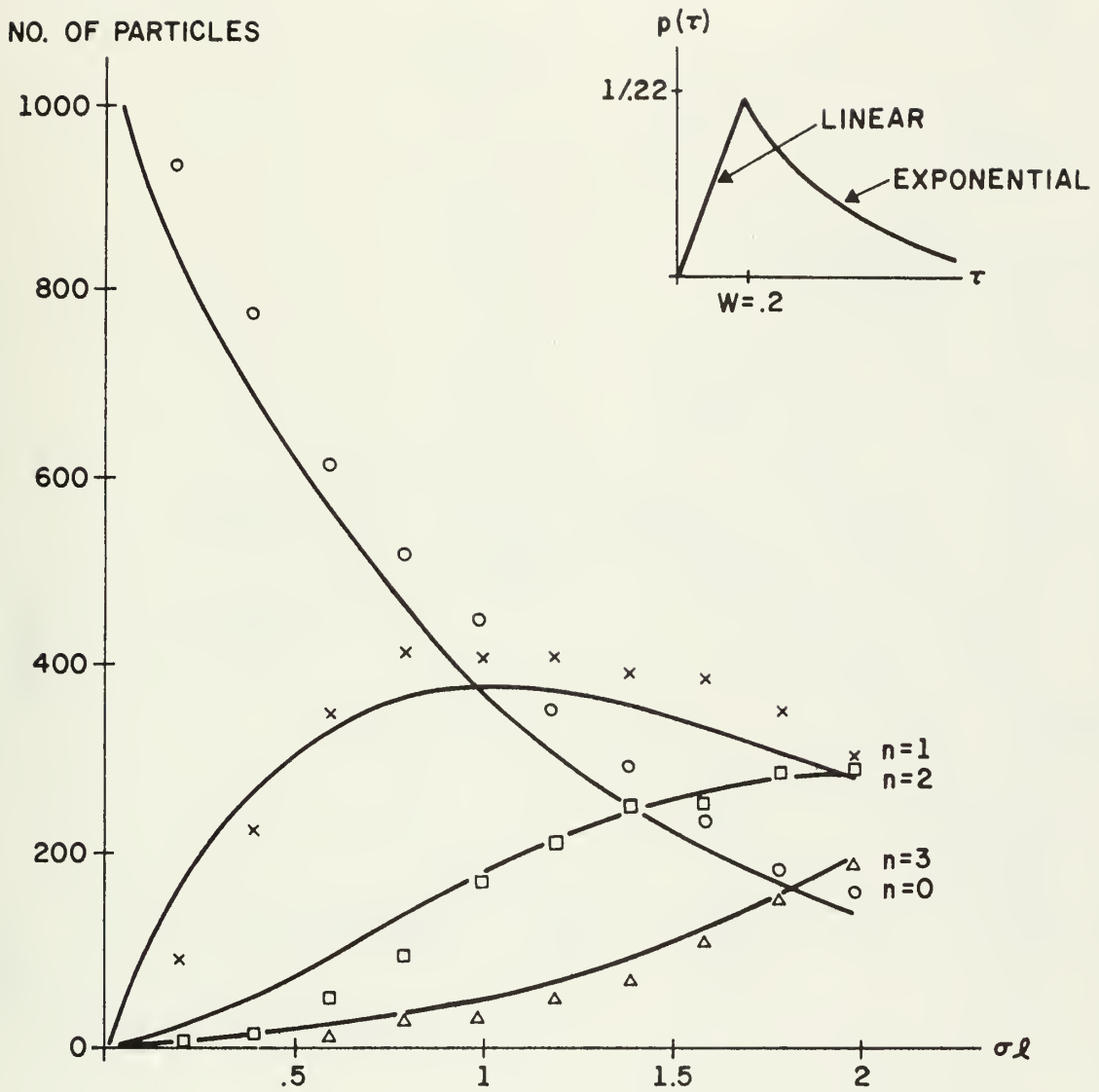


Figure 5.3 An Example of the Modified  $P(\tau)$  with  $W=0.2$   
 (above) and the Computational Results (below)  
 (Solid Curves are  $P_n(l) = \frac{(\sigma l)^n e^{-\sigma l}}{n!}$   $n=0, 1, 2, 3$ )

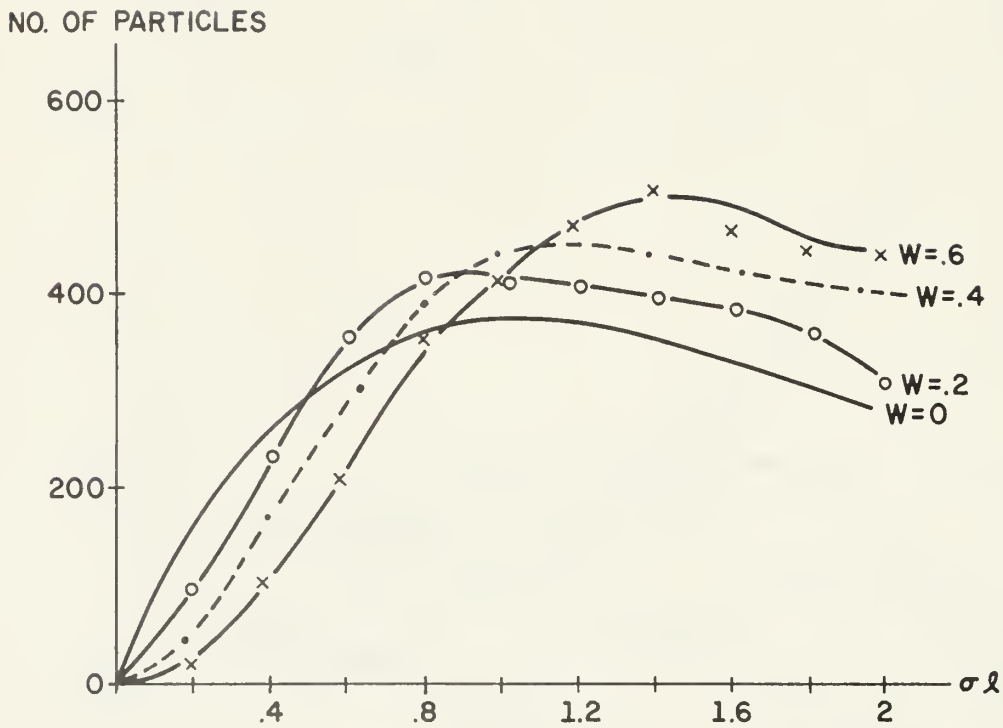


Figure 5.3 (continued) Comparison of Several  $P(\tau)$ s  
with Different  $W$ s ( $W=0,.2,.4,.6$ )  
(Only the Results for  $N=1$  are Displayed)

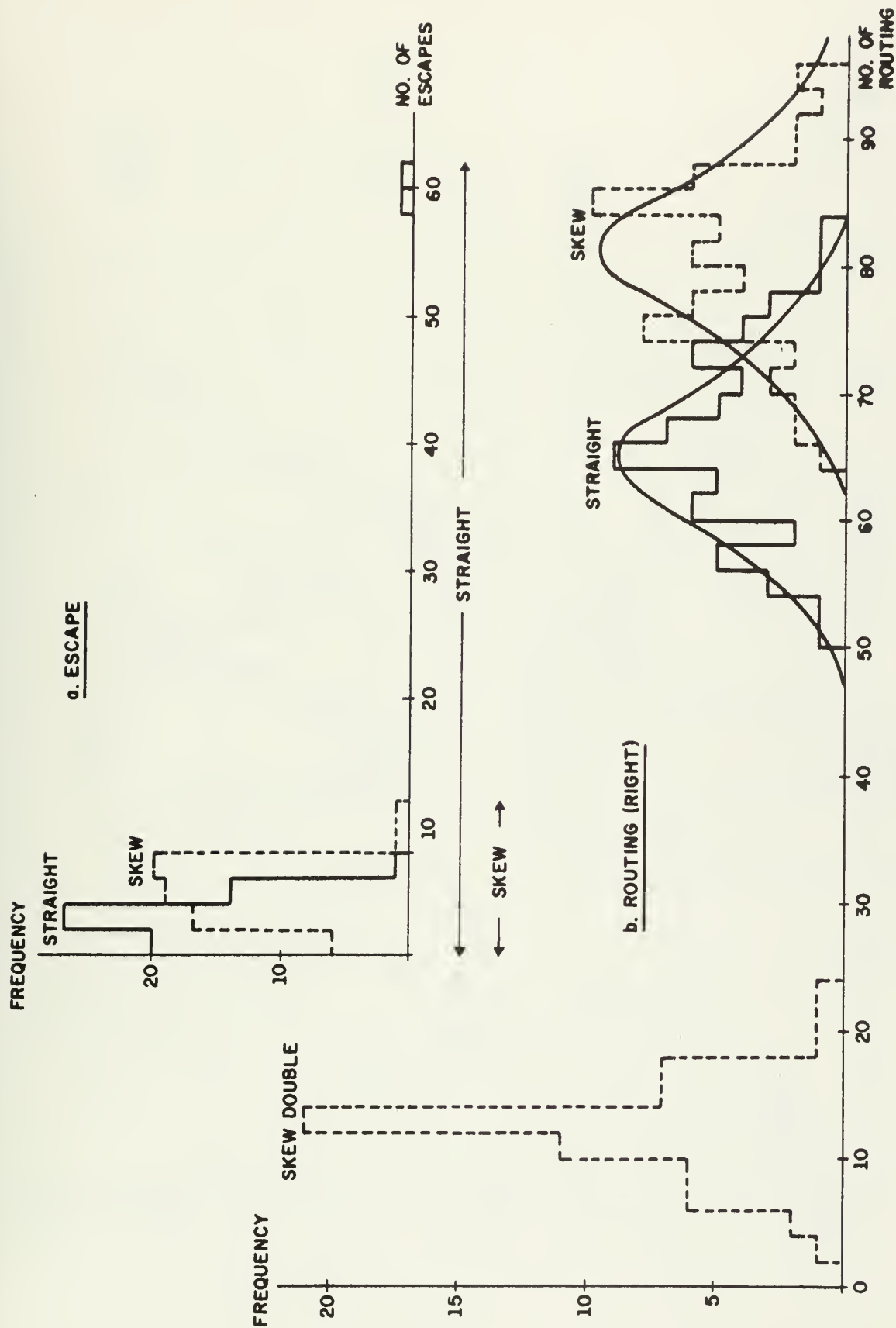


Figure 5.4 Straight Storage Vs Skewed Storage (64x8 Cells)  
 $\sigma=.4$ ,  $Vel.=1$ ,  $\Delta t=1$ , and  $\Delta x=1$ , 64x8x40 particles

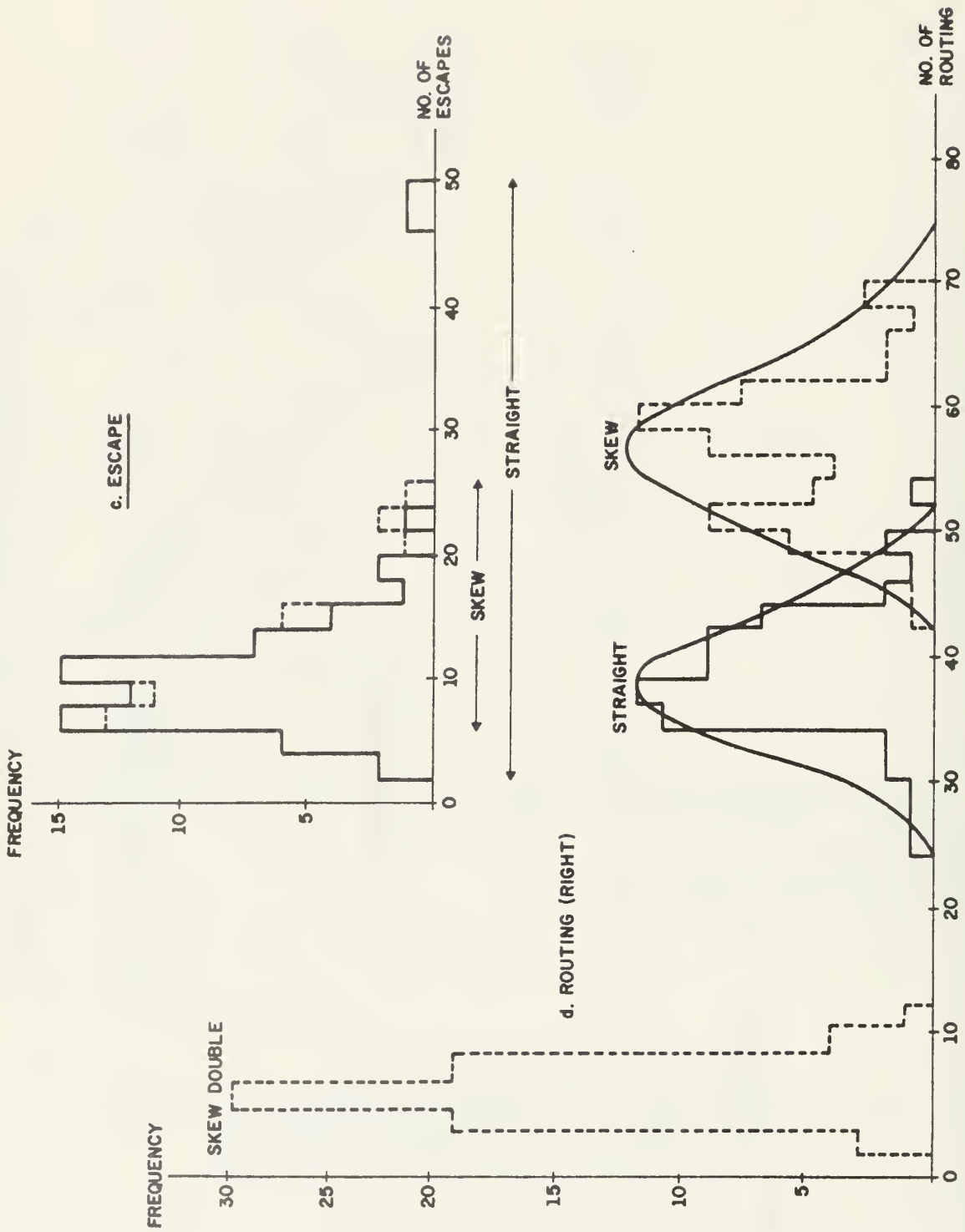


Figure 5.4 Straight Storage Vs Skewed Storage (64x8 Cells) (continued)  
 $\sigma=.2$ ,  $Vel.=.5$ ,  $\Delta t=1$ , and  $\Delta x=1$ , 64x8x40 particles



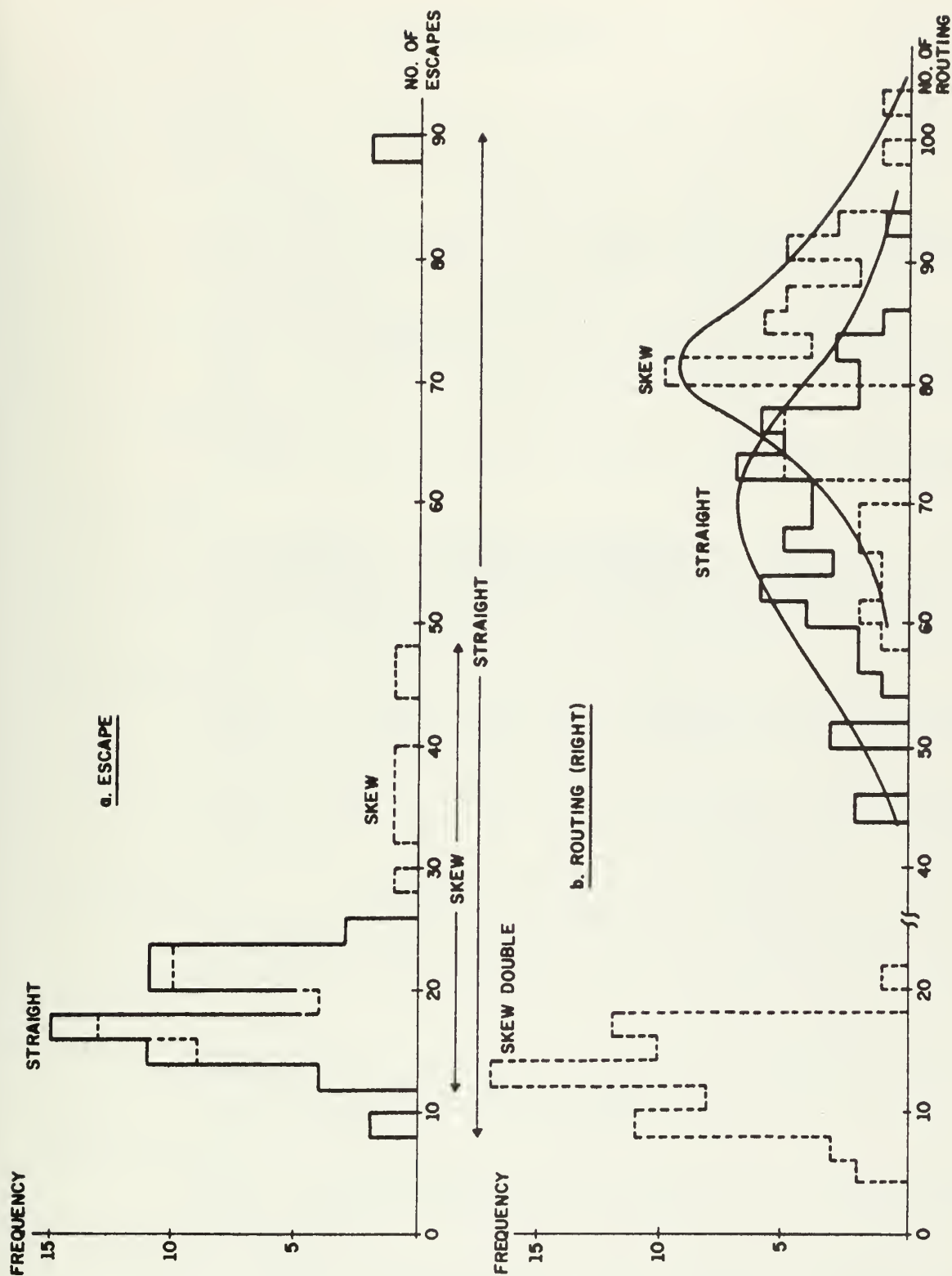


Figure 5.5 Straight Storage Vs Skewed Storage (64x64 Cells)  
 $\sigma=.4$ ,  $Vel.=1$ ,  $\Delta t=1$ , and  $\Delta x=1$ , 64x64x5 particles

	0	1-21	22-43	44-63
PKL		CNB	XCO	YCO
		MU	COS PHI	SIN PHI
	$\xi \Delta t$		ENERGY	
	WEIGHT		$\tau$	

	0-15	16-31	32-47	48-63
PNT	POINTER 1	POINTER 2	POINTER 3	POINTER 4

Figure 5.6 An Alternative Format for the Particle Table (not used in the test program)

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## APPENDIX 1

As is discussed in Chapter 3, it is interesting to investigate the probability density functions of the maximum length of chain-linked tables among PEs. Let the problem be stated as follows: There are  $N$  PEs and each PE has a table of  $M$  entries each of which is selected with the probability  $\sigma$  ( $0 < \sigma < 1$ ) so that the average length of the chains is  $\sigma M$ . What is the distribution of the maximum length of the chains? Assume that  $M$  is a large number and  $\sigma$  is neither too small nor too close to 1.

Theorem. If  $X_1, X_2$  have the distribution functions  $F_1(X), F_2(X)$  respectively, the distribution function of the stochastic variable  $X = \max(X_1, X_2)$  is  $F(X) = F_1(X)F_2(X)$ .

Proof. Let  $P_1(X), P_2(X)$  and  $P(X)$  denote the probability density functions of  $X_1, X_2$ , and  $X$ , respectively. Then,

$$\begin{aligned} P(X)dX &= P_1(X)dx \int^X P_2(X')dX' + P_2(X)dX \int^X P_1(X')dX' \\ &= P_1(X)F_2(X)dX + P_2(X)F_1(X)dX \\ &= \frac{d}{dX}(F_1(X)F_2(X))dX \end{aligned}$$

$$F(X) = F_1(X)F_2(X).$$

Q.E.D.

It is easy to derive the formula inductively when there are  $N$  independent variables. That is,  $X = \text{Max}(X_1, X_2, \dots, X_n)$  has the distribution function  $F(X) = F_1(X)F_2(X) \dots F_n(X)$  where  $F_i(X)$  is the distribution function of the  $i$ th variable.

Going back to the original problem, if the given assumptions are valid the distribution functions of the length of the chain in each PE can be approximated by the normal distribution:

$$\phi(X_i) = \frac{1}{\sqrt{2\pi M\sigma(1-\sigma)}} \exp \int_{-\infty}^{X_i} \exp \left\{ -\frac{(t-M\sigma)^2}{2M\sigma(1-\sigma)} \right\} dt \quad (i = 1, 2, \dots, N)$$

Therefore the distribution function of the maximum length  $\phi(X)$  is:

$$\phi(X) = \{\phi(X)\}^N \text{ or the probability density } P(X) \text{ is:}$$

$$P(X) = N \{\phi(X)\}^{N-1} \frac{1}{\sqrt{2\pi M\sigma(1-\sigma)}} \exp \left\{ -\frac{(t-M\sigma)^2}{2M\sigma(1-\sigma)} \right\}$$

Figure A1.1 shows  $P(X)$  for  $N(0,1)$  when  $N = 64$ .  $P(X)$  has the maximum value at  $X = 2.1$ . This was obtained by plotting values calculated from the mathematical table. (Ref. [16])

(Example)  $N = 64$  (ILLIAC IV)

$$M = 100$$

$$\sigma = .3$$

$$0 \leq Z \leq 100$$

$$\bar{Z} = 30$$

normalization of the variable

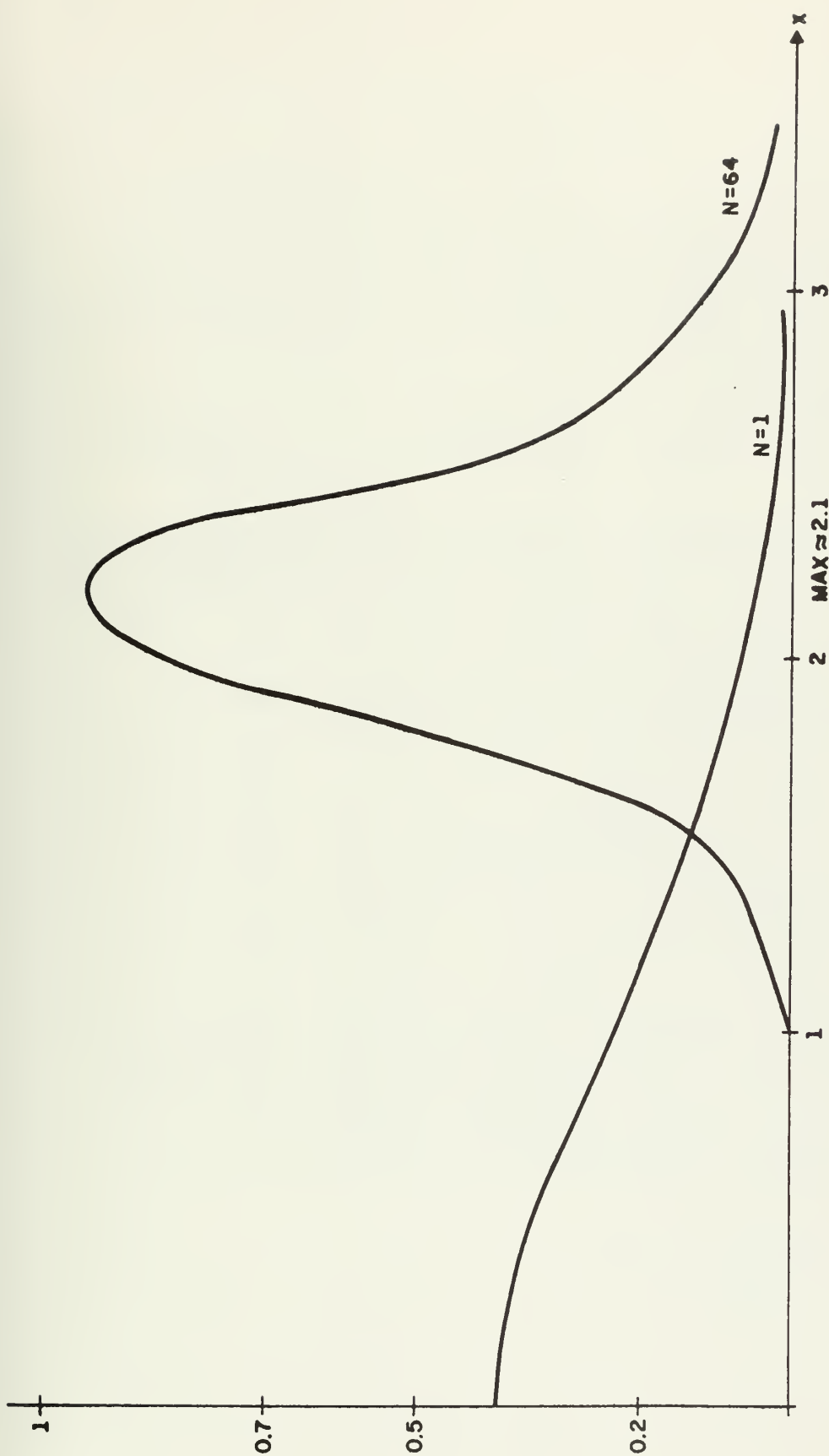
$$X = \frac{Z-30}{\sqrt{0.3 \times 0.7 \times 100}} = \frac{Z-30}{4.6}$$

$$X(Z = 100) = 15.2$$

$$X(Z = 0) = 16.5$$

$$Z(\text{peak}) = 30 + 2.1 \times 4.6 = 39.7$$

Therefore the expectation value of the maximum length of the chain is 40.



$$N=1: \text{NORMAL DISTRIBUTION } N(0,1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

**N=64: THE MAXIMUM VALUE OF 64 SAMPLES FROM N(0,1)**

Figure A.1 The Probability Density Function of the Maximum Value of 64 Samples from Normal Distribution

## APPENDIX 2

$P_n(\ell)$  in section 5.2 is derived in the following way:

Suppose  $n-1$  scatterings have happened in  $[0, x]$  and the  $n$ th scattering happens in  $[x, x+dx]$ . Then the probability that  $n$  scatterings happen anywhere in  $[0, \ell]$  is

$$P_n(\ell) = \int_0^\ell \underbrace{P_{n-1}(x)}_{\substack{\text{n-1 scattering} \\ \uparrow}} \cdot \underbrace{\sigma dx}_{\substack{\text{nth scattering} \\ \uparrow}} \underbrace{P_0(\ell-x)}_{\substack{\text{no scattering} \\ \uparrow}}$$

$$P_0(\ell) = \int_0^\ell \frac{1}{\sigma} e^{-\sigma x} dx = e^{-\sigma \ell}$$

Laplace transformation yields

$$\begin{aligned} q_n(s) &= \int_0^\infty e^{-s\ell} P_n(\ell) d\ell \\ &= \sigma q_{n-1}(s) q_0(s) \\ &= \sigma^n q_0(s)^{n+1} \end{aligned}$$

$$q_0(s) = \int_0^\ell e^{-s\ell - \sigma \ell} d\ell = \frac{1}{s + \sigma}$$

$$\therefore q_n(s) = \frac{\sigma^n}{(s + \sigma)^{n+1}}$$

Inverse Laplace transformation yields

$$\begin{aligned} P_n(\ell) &= \frac{\sigma^n}{2\pi i} \int_{C-i\infty}^{C+i\infty} \frac{e^{s\ell}}{(\sigma + s)^{n+1}} ds \quad (C > 0 \text{ real}) \\ &= \sigma^n \text{Res.}(s = -\sigma) \\ &= \frac{(\sigma \ell)^n}{n!} e^{-\sigma \ell} \end{aligned}$$

Q.E.D.





TM	•XXARESTIONAL TIME AS A FRACTION OF TMX	•	48
WT	•XXAFIGHTING FACTOR TO BE USED IN FREQUENCY	•	49
	•XXDEPENDENT CASE(WT+ENR IS THE ACTUAL ENERGY	•	50
	•XXCARRIED BY A PARTICLE).BECOMES ZERO AFTER	•	51
	•XXESCAPE OR ABSORPTION	•	52
ENR	•XXENERGY PER UNIT WEIGHT	•	53
SVD	•XXSURVIVAL DISTANCE (OR SO CALLED PATH LENGTH)	•	54
VEL	•XXVIRTUAL VELOCITY (PARTICLE DOES NOT GO AT	•	55
	•XXTHE VELOCITY OF LIGHT DUE TO SCALE ADJUSTMENT	•	56
AHC	•XXABSORPTION COEFFICIENT	•	57
SCC	•XXSCATTERING COEFFICIENT	•	58
DNS	•XXDENSITY OF MEDIUM IN WHICH A PARTICLE IS	•	59
	•XXTRAVELLING.(DEPENDS ON CELL NUMBER)	•	60
DUMMY	•XX DUMMY VARIABLE FOR RNIX (PHEAL)	•	61
SGM	•XX TOTAL CROSS SECTION OF INTERACTION	•	62
DLTS	•XX LENGTH FOR A PARTICLE TO TRAVEL IN DELTA T	•	63
RN	•XX CURRENT RANDOM NUMBER	•	64
ECTR	•XX ESCAPE COUNTER	•	65
ACTR	•XX ABSORPTION COUNTER	•	66
DGM	•XX DENSITY/TOTAL CROSS SECTION	•	67
	•XX(DIMENSION IS SAME AS SVD)	•	68
SPH	•XXSPECIFIC HEAT OF THE MEDIUM	•	69
SUM	•XX USED FOR SUMMING UP SOME OTHER VARIABLES	•	70
PCPOINT	•XXPARTICLE TABLE	•	71
DNFS	•XXDENSITY TABLE	•	72
ENERGY	•XXENERGY TABLE	•	73
CHECK	•XXUSED TO LABEL ROUTING,ESCAPE,INTERACTION, ETC.	•	74
	•XX X1:BOUNDARY CROSSING, X2:INTERACTION,	•	75
	•XX X3:ESCAPE, X4:ROUTING(+ OR -1)	•	76
REAL FIELD	X0(0,FULL)	•	77
	X1(0,INNER)	•	78
	X2(0,OUTER)	•	79
INTEGER FIELD		•	80
	X3(0,0,16)	•	81
	X4(0,16,16)	•	82
	X5(0,32,16)	•	83
	X6(0,48,16)	•	84
	X7(0,0,81)	•	85
	X8(0,8,8)	•	86
ALPHA FIELD	X(0,0,64)	•	87
		•	88
		•	89
*****		•	90
*****		•	91
SS	LIST OF SUBROUTINES	•	92
*****		•	93
		•	94
		•	95
		•	96
*****		•	97
	PREAL SUBROUTINE LN AS RGA(PHEAL X AS RGA)	•	98
*****		•	99
	BEGIN	•	100
8	INCINS 100		
88	TAPE2=GLYPNIR/GLN SERIAL;		
	END;*****NATURAL LOGXX	•	101
*****		•	102

```

103
PREAL SUBROUTINE EXP AS RGA(PREAL X AS RGA)
*****
      BEGIN
      INCINS      100
      ASKATCH=20
      TAPE2=GLYPNIR/GEXP SERIAL:
      END*****EXPONENTIAL***
*****
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108
PREAL SUBROUTINE SQR AS RGA(PREAL X AS RGA)
*****
      BEGIN
      INCINS      100
      ASKATCH=20
      TAPE2=GLYPNIR/GSQR SERIAL:
      END*****SQUARE ROOT***
*****
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PREAL SUBROUTINE SIN AS RGA(PREAL X AS RGA)
*****
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SUBROUTINE CHAIN(PINT OUT PCTR,PINT OUT PNTR,CINT Q,PINT
      PLOC)
*****
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PREAL SUBROUTINE CVTRL(PINT A AS RGA)
*****
      HOW TO USE THIS ROUTINE. SPECIFY AS FOLLOWS:
      SOME VARIABLE(CVTRL(PNT,II,X))
      THIS IS TO CONVERT 16 BIT INTEGER INTO 64 BIT REAL.

```

```

      BEGIN
        PREAL R AS R40,SS AS R05:
      S+
        SHAL 33:
      S+
        L05 34:
      S+
        SS.[115]=4000(4):
      S+
        L0A 35:
      S+
        N044:
        CVTRL=H:
      END: 48 CVTRL 44
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BEGIN  
 PREAL R AS R40,SS AS R05:  
 SHAL 33:  
 L05 34:  
 SS.[115]=4000(4):  
 L0A 35:  
 N044:  
 CVTRL=H:  
 END: 48 CVTRL 44

PREAL SUBROUTINE RNDX(CINT IV):  
 RANDOM NUMBER GENERATOR BY MIXED CONGRUENTIAL METHOD.  
 IF I<0 THEN INTEGER TYPE RANDOM NUMBERS ARE IN "RGLH".  
 IN THIS CASE RNDX IS ASSIGNED TO A DUMMY VARIABLE.  
 IF I<0 THEN REAL TYPE RANDOM NUMBERS ARE IN "RNOX".

BEGIN  
 PINT AA AS R04,BB AS R06,SS AS R05:  
 PREAL AA AS R04,SP AS R05:  
 AA=AA\* MULTIPLIER  
 R01=R04: R02=RNDX  
 RLM 3H:  
 AA=L0INST:  
 R01 34:  
 RGLH=AA: RNDX=RNDX (INTEGER)  
 IF I<0 THEN  
 BEGIN  
 L05 34:  
 SP.[115]=4000(4): CONVERSION TO REAL TYPE  
 L0A 35:  
 N044:  
 RNDX=AA:  
 END:  
 END: 48 RNDX 4

SUBROUTINE DATALD:  
 BEGIN  
 PREAL  
 TEMP:  
 SIMHEAD(CARD,HGLF): \*\*\*HEAD INITIAL RANDOM NUMBER  
 SIMHEAD(CARD,ABC,SEC,THX,STP):  
 TAUP1=6.2431553071740:  
 LOOP 11=0.1,7 10  
 BEGIN  
 SIMHEAD(CARD,TEMP):  
 DENS.[1]X1=TEMP: DENSITY  
 SIMHEAD(CARD,TEMP):  
 ENERGY.[1]X1=TEMP: TEMPERATURE  
 SIMHEAD(CARD,TEMP):  
 DENS.[1]X2=TEMP: ASPECTIC HEAT  
 ENERGY.[1]X2=0: \*\* TALLY CLEARED.  
 END:

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END: XDATALOAD
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      PKL.(SNXT)X6:=COS(THETA)*16344J
      PKL.(SNXT+1)X1:=P4DX(1)+TNAJ
      PKL.(SNXT+2)X2:=-LN(1-MV)X(1))J
      SNXT:=PKL.(SNXT+1)X4J
      ENDJ
      SCITH:=0J
      ENDJ  XXIRTH
      22J
      20J
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE TALLYJ
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN
      X      SUM UP THE PARTICLES IN EACH CELL.
      X
      X      LOOP TNR:=1,4,76 J
      X      BEGIN
      X      DPTH:=MUJ(PKL.(TNR)X3J)
      X      ENERGY.(DPTH)X1:=ENERGY.(DPTH)X1+PKL.(TNR+2)X2*
      X      PKL.(TNR+3)X1J
      X      ENDJ
      X
      X      ENDJ  XX TALLY  XX
      25J
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE ENERGYBALANCEJ
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN
      X
      X      THIS SUBROUTINE IS TO CALCULATE THE NEW ENERGY AND THE
      X      RADIATION IN THE NEXT STEP. THIS SUBROUTINE SHOULD BE
      X      CALLED AFTER PROCESSING PARTICLES, AND IS TO BE FOLLOWED
      X      BY "PARTICLEASSIGN".
      X
      X      GLOBAL VARIABLES ARE
      X      PREAL  ISPH(SPECIFIC HEAT IN CGS UNIT.)
      X      STP (STEPHAN-BOLTZMANN'S CONSTANT FOR BLACK BODY
      X      RADIATION, IN CGS UNIT.)
      X      SUM (TO TAKE SUM OF RADIATIVE ENERGY.)
      X      CINT  ITMX (LENGTH OF TIME STEP.)
      X      PINTFRJ
      X      ENERGY (STORED ENERGY IN EACH CELL)
      X      DENS (DENSITY OF EACH CELL)
      X      CFAV (FREQUENCY-AVERAGED ABSORPTION COEFFICIENT)
      X
      X
      X      CINT  DPTHJ
      X      PREAL  XY,XZJ
      X      CREAL  CFAVJ
      X      CFAV:=ABCJ
      X      SUM:=0J
      X      LOOP DPTH:=0,1,7 J
      X      BEGIN
      X      XZ:=ENERGY.(DPTH)X1J
      X      SPH:=DENS.(DPTH)X2J
      X      XY:=XZ/SPHJ
      X      XY:=XY*XYJ
      X      X STORER ENERGY READ OUT
      X      X SPECIFIC HEAT
      X      X TEMPERATURE
      X      X TEMP ***
      X

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```

      XYI=XY+XYI
      DGM1=CFAY+STP+THY+DENS.(DPTH)X1
      XYI=UGM+XYI
      XZ1=XZ-XY+DGM+ENERGY.(DPTH)X2I
      ENERGY.(DPTH)X1=XZ1  ** STORED ENERGY OF THIS CELL.
      ENERGY.(DPTH)X2=XZ1  ** RADIATIVE ENERGY
END** LOOP **
      SUMI=SUM+XYI

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FNDI \*\* ENERGYBALANCE \*\*

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*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*
SUBROUTINE PARTICLEASSIGN:
*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*
      BEGIN

```

THIS SUBROUTINE IS TO DISTRIBUTE PARTICLE TABLE TO CELLS.  
ENERGY DISTRIBUTION IS NOT CONSIDERED. ENERGY IS CONSERVED.  
CELL NUMBERS OF PARTICLES ARE ALSO ASSIGNED HERE. VACANCY  
CHAIN IS TRANSFERRED TO SCATTER CHAIN TO CONNECT ALL NEW PARTICLES.

GLOBAL VARIABLES ARE:

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      PREAL:
      SUM (SUM OF RADIATIVE ENERGY IN EACH PF)
      PINT:
      VNAT (VACANCY POINTER)
      VCTR (VACANCY COUNTER)
      SNAT (NEW PARTICLE POINTER)
      SCIN (NEW PARTICLE COUNTER)
      PCTR (NUMBER OF TABLE ENTRIES AVAILABLE FOR NEW
      PARTICLES)
      POINTERS:
      ENERGY (STORED ENERGY TABLE).
      PKL (PARTICLE TABLE)

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      PINT J,K,THP,PNT
      CINT DPTH1  X(NH1) GLOBALLY DPTH1 IS PE INTERGER.
      PREAL XY,XZ1
      PCTR=VCTR+.6671  XY ONLY 2/3 OF THE VACANCY IS
                      USED FOR NEW PARTICLES.
      LOOP DPTH1=0.1.7 DO
      BEGIN
      KI=ENERGY.(DPTH1)X2/SUM+PCTR1  ** INDICATED TABLE
                      ** ENTRIES ARE ASSIGNED
                      ** TO THIS CELL.
      SIMWRITE(LINE,"K=",K)
      FOR PNB1=1 STEP 1 UNTIL K DO
      BEGIN
      PKL.(VNAT)X31=PFN+A+DPTH1  ** CELL NUMBER
      PKL.(VNAT+3)X11=11  ** WEIGHTING FACTOR
      PKL.(VNAT+2)X21=XZ/PCTR1
                      ** ENERGY IS ASSIGNED TO
                      ** A PARTICLE IN MONO-
                      ** CHROMATIC CASE. THAT

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*****
SUBROUTINE ESCAPE1
*****
THIS SUBROUTINE IS TO TREAT PARTICLES WHICH ESCAPE OUT OF THE
MEDIUM, TABLES FOR THOSE PARTICLES ARE DESTROYED AND THE
COUNTER IS INCREMENTED BY EIGHT.

      BEGIN
          FCTR1=ECTR+NT;
          CHECK,X51=4096;
          NT=0;
          CHAIN(VCTR,VNXT,TJH,0);
      END;  **ESCAPE FROM THE MEDIUM
*****
*****
SUBROUTINE ABSORB1
*****
      BEGIN
          ACTR1=ACTR+NT;  **ABSORPTION COUNTER INCREMENTED.
          NT=0;          **TO IDENTIFY AN ABSORBED PARTICLE
          CHAIN(VCTR,VNXT,0,TJH);
      END;  **ABSORB 1
*****
*****
SUBROUTINE TRANSLATE1
*****
      BEGIN
*****
THIS SUBROUTINE HAS TWO FUNCTIONS. ONE IS TO TRANSLATE
PARTICLES TO NEW POSITIONS ACCORDING TO VELOCITY, DIRECTION
COSINE. THE OTHER IS TO DETECT PARTICLES WHICH CROSS CELL
BOUNDARIES OR THOSE WHICH ESCAPE FROM THE MEDIUM AND
TO LABEL THEM USING CHECK,X6 (ROUTE CHECK) AND CHECK,X7 (
ESCAPE CHECK), RESPECTIVELY.

THIS SUBROUTINE IS TO BE IMMEDIATELY IN SUBROUTINE BRANCH.

      PREL
          /;
          XCU1=XCU+DLTS*MU1;  **XCD INCREMENTED
          YCU1=YCU+DLTS*SURT(1-MU*MU1)*SNF;  **YCU INCREMENTED
          TM1=TM-DLTS/VEL;  **TIME DECREMENTED
          SVD1=SVD-DLTS*UGM;  **SURVIVAL DISTANCE DECREMENTED
*****
*****
          Z1=XCU1
          FOR ALL Z GEQ .9999 DO
              BEGIN
                  XCU1=0;

```



SUBROUTINE BRANCH(PINT TNR))	506
*****	507
BEGIN	508
THIS SUBROUTINE IS TO DECIDE WHAT INTERACTION IS TO TAKE PLACE.	509
AFTER THAT TRANSLATE IS CALLED, THEN ROUTE LINKING IS PERFORMED.	510
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PREFAL XY,XZ,XW:	520
L131	521
CHECK.X3:=0:	522
FOR ALL CHECK.X5=4192 DO	523
BEGIN	524
CHECK.X5:=4096:	525
OSTND:	526
DLTS:=VEL*TN:	527
XY:=DHR-DLTS:	528
DGM:=(CHECK.X3)DMS.(DEPTH)*X1+SG*:	529
XZ:=SVD-DLTS*DGM:	530
XW:=DGM-DHR-SVD:	531
FOR ALL XY<0 AND XW LEQ 0 DO PROCESSING BOUNDARY	532
BEGIN	533
CHECK.X5:=4192:	534
DLTS:=DHR:	535
END:	536
FOR ALL XY GEQ 0 AND XZ<0 OR XY<0 AND XW>0 DO	537
BEGIN INTERACTION	538
DLTS:=SVD/DGM:	539
CHECK.X6:=4096:	540
END:	541
538	
THOSE ARE TO HAVE INTERACTION	542
TRANSLATE:	543
544	
GO TO L131	545
END:	546
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524	
FOR ALL CHECK.X7=1 DO	549
ESCAPE:	550
FOR ALL CHECK.X3=1 DO WRIGHT ROUTING	551
CHAIN(HCTH,RNXT,1,TNR):	552
FOR ALL CHECK.X3=-1 DO	553
CHAIN(LCTH,LNXT,1,TNR):	554
THOSE ARE FOR "ESCAPE"	555
CHECK.X8:=0:	556
CHECK.X5:=4096:	557
FOR ALL CHECK.X6=4096 AND WT>.01 DO INTERACTION TYPE	558
BEGIN	559

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      XYI=AMC/SGMI
      NNI=RNDX(1)
      FOR ALL NN LEO XY DO
        ABSINN:
      FOR ALL NN XY DO
        CHAIN(SCTH,SNXT,0,TNR)) SCATTERING
      ENDS INTERACTION
55)
*
      SIMWRITE(LINE,"BRANCH CALLED","ESCK=",CHECK,7,
        "RTCK=",CHECK,XA)
      ENDS BRANCH
56)
*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE STORE(PINT IN)
*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN
      TO STORE DATA ON A PARTICLE TO PARTICLE TABLE
      PKL.(TNH)X3I=CNH: XCELL NUMBER
      PKL.(TNH)X5I=XCN+16384: XCOORDINATE
      PKL.(TNH)X6I=YCN+16384: XYCOORDINATE
      PKL.(TNH+1)X5I=MCN+16384: XDIRECTION COSINE
      PKL.(TNH+1)X6I=SNF+16384: XSIN OF AZIM.ANGLE
      PKL.(TNH+1)X6I=CSF+16384: XCOS OF AZIM.ANGLE
      FOR ALL CHECK,XA NEQ 4096 AND WT NEQ 0 DO
      PKL.(TNH+2)X1I=1: XDELTA T.
      PKL.(TNH+3)X1I=WT: XWEIGHT
      PKL.(TNH+3)X2I=SDI: XSURVIVAL DISTANCE
      ENDS STORE
57)
*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE ANGLE
*****XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      DETERMINATION OF SCATTERING ANGLES, DIRECTION COSINE OREYS
      THE LAW OF THOMPSON SCATTERING, I.E. PROH(MU)=3/81(1+MU/MU),
      AZIMUTHAL ANGLE IS UNIFORM.
      BEGIN
      PREAL XX,XY,XZ,XW,T1,T2,T3,THETA,KI
      CINT I
      XA RANDOM NUMBER WITH THE PROH. DENSITY GIVEN ABOVE
      XYI=.7: XINITIAL VALUE OF NEWTON-RAPHSON'S METHOD
      XW1=RNDX(1)
      I DOUP I=1,1,3 ON XNEWTON-RAPHSON ITERATION
      BEGIN
      XZ1=XY+XY
      XYI=(XY+XZ+.5-XW)*1.333333/(1+YZ)
      ENDS
      KI=XY: XSCATTERING ANGLE (DIRECTION COSINE)
      THETA1=THNPI+RNDX(1): XAZIM.ANGLE
      XW1=SQRT(1-KI+KI): XSIN(KI)
      XX1=SQRT(1-MU+MU): XSIN(ORIGINAL DIRECTION)
      XZ1=XW+XX
      CALCULATION OF NEW DIRECTION COSINE AND AZIMUTHAL ANGLE OF PARTICLES.

```

```

FOR ALL XN NEW 0 DO
  BEGIN
    XYI=MU*KI-XI*COS(THETA);
    T1I=SQRT(1-XYI*XYI);
    FOR ALL T1 NEW 0 DO      * NEW SET OF AZIM.
      BEGIN
        T2I=XW*SIN(THETA)/T1I;
        T3I=(MU*XY-KI)/(XI+T1I);
        T1I=CSFI;
        CSFI=T2I*SNF+T3I*CSFI;
        S4FI=T3I*SNF-T2I*T1I;
      ENDI
    ENDI
  ENDI
  BEGIN
    SNFI=SIN(THETA);
    CSFI=COS(THETA);
  ENDI
  MUJ=XYI;
  XWI=RNDX(1);
  FOR ALL XW>.5 DO
    MUJ=-MUJ;
  ENDI
  * NEW ANGLES
  BEGIN
    THOMSON SCATTERING NEW DIRECTION COS. AZIM. ANGLES, TM AND SURVIVAL
    DISTANCE ARE SELECTED
    PRINT TNRI;
    PRFAL THETA;
    LABEL LSI;
    SIMWRITE(LINE,"SCATTERING CALLED");
    SIMWRITE(LINE,"SCATTERED PARTICLE=","SNXT");
    LSI: FOR ALL SCTX>0 DO
      BEGIN
        CNB)=PKL.(SNXT)X3;  * CELL NUMBER
        DPTHI=MJD(CNB);
        YCUI=CVTRL(PKL.(SNXT)X5);
        YCUI=CVTRL(PKL.(SNXT)X6);
        ANGLEI;
        TM)=PKL.(SNXT+2)X1;
        DGM)=DENS.(DPTH)X1+SGM;
        FNR)=PKL.(SNXT+2)X2;
        WT)=PKL.(SNXT+3)X1;
        SVD)=LN(1-RNDX(1));
        FOR ALL WT GEQ .01 DO
          CHECK.A5I=H192;  * ENABLE PEIS IN "BRANCH"
          BRANCH(SNXT);
        ENDI
      ENDI
    ENDI
  ENDI

```

```

      PKL, (SNXT+2)X1:=TMJ
      CHECK,XA1:=4094J
      STORE(SNXTJ)
      SNXT:=PKL, (SNXT)X4J
      SCTR:=SCTP-1J
      GO TO LSJ
    ENDJ
  65J
ENDJ  %SCATTERING
  66J
  67J
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      AI=CVTRL(PKL.(II+1)X5)      * 719
      SIMWRITE(LINE,"DIRECTION COS",A)      * 720
      SIMWRITE(LINE(PAGE),"POINTER 1",PKL.(II)X4)      * 721
      SIMWRITE(LINE,"POINTER 2",PKL.(II+1)X4)      * 722
      AI=CVTRL(PKL.(II)X5)      * 723
      SIMWRITE(LINE(PAGE),"X=COORDINATE",A)      * 724
      AI=CVTRL(PKL.(II)X6)      * 725
      SIMWRITE(LINE,"Y=COORDINATE",A)      * 726
      AI=CVTRL(PKL.(II+1)X3)      * 727
      SIMWRITE(LINE(PAGE),"SIN PFI",A)      * 728
      AI=CVTRL(PKL.(II+1)X6)      * 729
      SIMWRITE(LINE,"COS PFI",A)      * 730
      SIMWRITE(LINE(PAGE),"DELTA T",PKL.(II+2)X1)      * 731
      SIMWRITE(LINE,"ENERGY",PKL.(II+2)X2)      * 732
      SIMWRITE(LINE(PAGE),"SURVIVAL DIST.",PKL.(II+3)X2)      * 733
      SIMWRITE(LINE,"HEIGHT",PKL.(II+3)X1)      * 734
      ENDI  X PRINT PARTICLE TABLE      * 735

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X      * 736
X      * 737
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 738
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 739
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 740
X      * 741
      BEGINNING OF MAIN PROGRAM      * 742
X      * 743
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 744
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 745
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX      * 746
      PKL1=GETPER(80)      * 747
      DENS1=GETPER(8)      * 748
      ENERGY1=GETPER(8)      * 749
      CHECK1=GETPER(1)      * 750
X      * 751
X      * 752
      DATALOADS      * 753
      SGM1=ABC+SCC      * 754
X      * 755
XX     COUNTERS CLEARED      * 756
      ACTRI=0      * 757
      ECTRI=0      * 758
      VNXTI=0      * 759
      VCTRI=0      * 760
      LOOP TNR1=0,4,76 DO      X 20 PARTICLES IN EACH PF.      * 761
      CHAIN(VCTR,VNXT,0,1NB)  X VACANCY IS LINKED.      * 762
X      * 763
X      * 764
      LOOP TIME1=0,1,3 DO      X BEGINNING OF TIME CYCLE      * 765
      BEGIN      * 766
      RCTRI=0      * 767
      LCTRI=0      * 768
      RNXTI=1      * 769
      LNXTI=1      * 770
X      * 771
X      * 772
      ENERGYBALANCE      * 773
      PARTICLEASSIGN      * 774

```



BIRTH;		•	775
LOOP TNR=0,1,76 DO	%BEGINNING OF TABLE SCANNING	•	776
HERIN		•	777
%\$ READ OUT FROM THE PARTICLE TABLE %\$		•	778
CNR=PKL.(TNR)X3;	% CELL NUMBER	•	779
XCU=CVTRL(PKL.(TNR)X5);	% X-CO ORDINATE	•	780
YCU=CVTRL(PKL.(TNR)X4);	% Y-COORDINATE	•	781
TNR=TNR+1;		•	782
MU=CVTRL(PKL.(TNR)X9);	%DIRECTION COSINE	•	783
SFI=CVTRL(PKL.(TNR)X3);	%SIN PHI	•	784
CFI=CVTRL(PKL.(TNR)X4);	%COS PHI	•	785
TNR=TNR+1;		•	786
TM=PKL.(TNR)X1;	%RESIDUAL TIME	•	787
ENR=PKL.(TNR)X2;	%ENERGY	•	788
TNR=TNR+1;		•	789
WT=PKL.(TNR)X1;	%WEIGHTING FACTOR	•	790
SUI=PKL.(TNR)X2;	%SURVIVAL DISTANCE	•	791
DPTH=MOD(CNR);		•	792
FOR ALL AT GF, .01 DO		•	793
CHECK.X51=8192;	%ENABLE PEIS IN BRANCH	•	794
BRANCH(TNR);		•	795
STORE(TNR);		•	796
CHECK.X71=0;		•	797
END;	% TABLE SCANNING	•	798
		•	799
		•	800
SCATTER;		•	801
ROUTE(RCTR,RNXT,1);		•	802
ROUTE(LCTR,LNXT,03);		•	803
TALLY;		•	804
END; %TIME CYCLE		•	805
END, % OF MAIN		•	806

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1



\*\*\*\*\*APPROXIMATE PROGRAM SIZE\*\*\*\*\*

S	INSTRUCTION SYLLABLES GENERATED.....	3383
S	BOOLEAN STORAGE.....	10 WORDS PER QUADRANT
S	CU REGISTER STORAGE.....	25 WORDS
S	PE REGISTER STORAGE.....	4444 WORDS PER QUADRANT
S	MISCELLANEOUS.....	3600 WORDS
S	***** TOTAL.....	13766 WORDS

CONGRATULATIONS. NO SOURCE PROGRAM ERRORS WERE DETECTED.

TOTAL TIME..... 1:12  
 CPU TIME..... 0:39  
 I/O TIME..... 0:28  
 806 CARDS PROCESSED AT 1211 C.P.M. (CPU)



UNCLASSIFIED

Security Classification

## DOCUMENT CONTROL DATA - R &amp; D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

## 1. ORIGINATING ACTIVITY (Corporate author)

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A MONTE CARLO METHOD APPLIED TO ILLIAC IV AND ITS STATISTICAL CONSIDERATION

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## 13. ABSTRACT

A Monte Carlo method to solve radiation transport problems by using the ILLIAC IV is discussed. An emphasis is put on the special features to be encountered in parallel computation: data structure, PE efficiency, etc. A test program implemented in GLYPNIR--an ILLIAC IV language--is shown and some preliminary results on its statistical properties are also discussed.

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